OPTIMAL DESIGN AND RETROFIT OF THREE PRODUCT DIVIDED WALL COLUMN

BY

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Dedicated to my beloved parents, brothers, all teachers who have been there for my guidance ever since I started my education and friends

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LIST OF ABBREVIATIONS

DWC	:	Divided Wall Column
FTCDC	:	Fully Thermally Coupled Distillation Column
PTCDC	:	Partially Thermally Coupled Distillation Column
C2C	:	Conventional two Column system
BTX	:	Benzene, Toluene and p-Xylene
BTE	:	Benzene, Toluene and Ethyl-benzene
NRTL	:	Non Random Two Liquid Model
SRK	:	Soave-Redlich-Kwong Model
UNIQUAC	:	Universal Quasi Chemical Model
VLE	:	Vapor Liquid Equilibrium
CEPCI	:	Chemical Engineering Plant Cost Index
MSI	:	Marshall & Swift Cost Index
TAC	:	Total Annual Cost
TIC	:	Total Installed Cost

ABSTRACT

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Distillation is a commonly used unit operation for separating multicomponent liquid mixtures in chemical process industries and it is very energy intensive process. Among the various types of distillation column, the divided wall column (DWC) is currently the most energy efficient distillation column for multicomponent separation. The divided wall column is currently receiving a lot more attention from the industry due to its superior energy performance and low investment cost.

The design and operation of the DWC is more complex than the conventional distillation column system. In this study, an efficient design method has been proposed to determine the optimal design structure of a DWC based on extensive simulation study. The initial design parameters of the DWC have been fixed on the basis of shortcut method (Fenske-Underwood-Gilliland method). The rigorous optimization approach is used to obtain the optimal design parameters of DWC using Aspen HYSYS.

To analyze the effectiveness of the proposed design procedure, four different ternary feed mixtures are used. The obtained results show that an optimal design structure could save a significant amount of energy, up to 35%, compared with the nominal design based on a shortcut method. A simulation study has been performed to study the effect of the variable feed composition on thermal efficiency of the DWC and the results shows that the DWC

thermal efficiency increases as the concentration of the middle component in the feed increases. A detailed economic evaluation of an optimized DWC based on minimum energy consumption is carried out and results indicate that the DWC is economically attractive, as it reduces the operating cost by up to 35% and the capital cost by up to 18% compared with a conventional column. An analysis has also been performed to investigate the effect of the energy supply on the product compositions.

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عنوان الرسالة: التصميم الأمثل و رفع كفاءة عمود تقصير ذو جدار فاصل لتقطير ثلاث مواد كيميائية

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عملية التقطير أو الفصل هي عملية شائعة الاستخدام في معامل تكرير النفط و تصنيع البتر وكيماويات و تستخدم أعمدة التقطير لفصل عدة منتجات كيميائية حيث تستلزم هذه العملية كمية كبيرة من الطاقة. و هناك أنواع كثيرة من أعمدة و طرق التقطير من أحدثها و أقلها استهلاكا للطاقة ما يعرف بعمود التقطير ذو جدار التقسيم و هو محط أنظار كثير من الدراسات الحديثة لقدراته على فصل عدة مواد و كذلك لتوفيره للطاقة.

و يعد تصميم و تشغيل مثل هذه الأعمدة تحدياً كبيراً مقارنة بأعمدة التقطير التقليدية. في هذه الدراسة، تم اقتراح طريقة تصميم فعال لتحديد التصميم الأمثل لعامود تقطير ذو جدار مقسم بناء على دراسة محاكاة واسعة النطاق و على أساس طريقة الاختصار المعاملات فنسك أندروود جيليلند (Fenske-Underwood-Gilliland). يتم استخدام برنامج المحاكاة هايسس (HYSYS) لتحديد أفضل تصميم لعامود التقطير.

و لتحليل فعالية التصميم الداخلي المقترح، تم محاكاة عملية فصل أربع مجموعات أو مخالط مختلفة من المواد الكيميائية في كل مجموعة تمم فصل ثلاثة منتجات بنسب عالية كما هو مطلوب بالصناعة و الأسواق. . وتظهر النتائج أن هيكل التصميم الأمثل يمكن أن يوفر كمية كبيرة من الطاقة تصل إلى 35٪

كما أن تكلفة الاستثمار انخفضت بنسبة 18%. كما توضح الدراسة العلاقة بين الطاقة المستخدمة لعملية الفصل مع تركيز المواد المفصولة.

CHAPTER 1

INTRODUCTION

Distillation is the common thermal separation technique used for separating multicomponent liquid mixtures into its desired purity level by the application and removal of heat (vaporization and condensation). This separation technique is based on differences in relative volatilities of different components. Distillation process is one of the best preferred methods of separation in the process industry like gas processing, refineries, petroleum, chemical and petrochemical units. As research continues for better alternative, the distillation process has also been improving. Breakthroughs have been made from time to time which has enhanced the level of the sophistication of distillation process, but it still remains very energy-intensive process.

Distillation alone accounts for the major part of energy usage in process industries due to cooling and heating involved through condenser and reboiler to achieve the desired product purities [1]. Distillation consumes almost 3% of the world's energy consumption [2]. It is noted that more than 65% of the total operating cost of the plant consists of energy expenditures [3]. In current scenario, all the industries including process industries are bearing globalization and international competition to achieve reduced manufacturing cost. Motivated by high energy consumption for distillation, different strategies have been proposed by different researchers to enhance the energy performance in distillation

process. Any kind of energy savings will not only results in profitability of the process but it also reduces the excessive CO_2 emission in the environment.

1.1 Emergence of Divided Wall Column (DWC) Structure

Almost in every industry around the world, product cost is being increased in result of increasing energy cost due to escalation in oil prices. Distillation alone accounts for the significant amount of world's energy consumption and it is used for 94% of total liquid separations in petrochemical and other related process industries [4]. Literature indicates that distillation uses 55% to 75% of energy and capital cost of a traditional chemical process, so any developments in distillation technology could be added to the process industries. Distillation demands large amount of energy consumption, therefore many researchers have proposed different energy efficient separation approaches for saving of energy and capital cost.

For minimization of energy usage and capital cost, it is necessary to study the different column configurations in order to select a best possible arrangement for particular separation by distillation technique.

Different Types of Distillation Column Schemes

Various column schemes have been established to minimize the energy demands of conventional distillation system. There are simple and complex distillation column configurations. Both the simple column and complex column arrangements are discussed here in details.

1.2 Simple Column Configurations

Simple distillation column arrangements are well known in industries and are conventional, they include direct column, indirect column and distributed column sequences. These conventional sequences of distillation are simple in operation and design to get the desired product purity in multi-component system. This configuration consists of two or more columns connected by a single supply stream. For ternary feed mixture, the possible simple column sequences are the following:

1.2.1 Direct Column Sequence

It consists of configurations that separate the light product in the first column as a distillate stream and the heavy components are fed through the bottom of 1st column to next column for further separation (Figure 1-1). Both columns are separated from each other by a single stream and they must be operated at different pressure to carry out the sharp separation.

Direct column sequence is used when ternary feed mixture contains high amount of light component (upto 80%) in it or when the fractionation between the middle and the heavy component is complex as compare to the separation of lighter product and middle product.

1.2.2 Indirect Column Sequence

It consists of configurations in which the heaviest product is separated from the bottom of first column as a bottom product and the other light products are obtained as a pure component in the subsequent column (Figure 1-2). Indirect sequence is utilized when the ternary feed mixture contains large amount of heavy components or when the separation of the lighter product from the middle product is difficult. In this sequence, the last column

usually operates at low pressure than that of the previous column to ensure the flow of the vapors naturally from one column to the other column, otherwise there will be a need of compressor between columns.

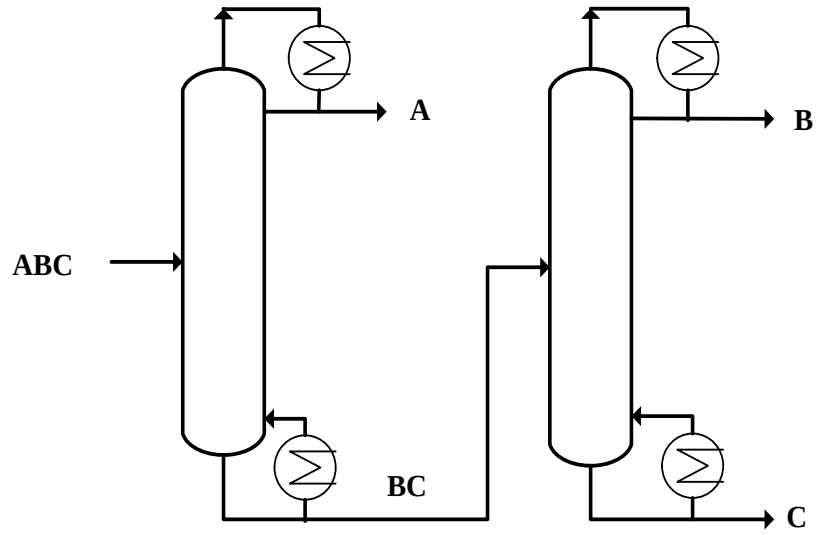


Figure 1-1: Direct Distillation Column Sequence

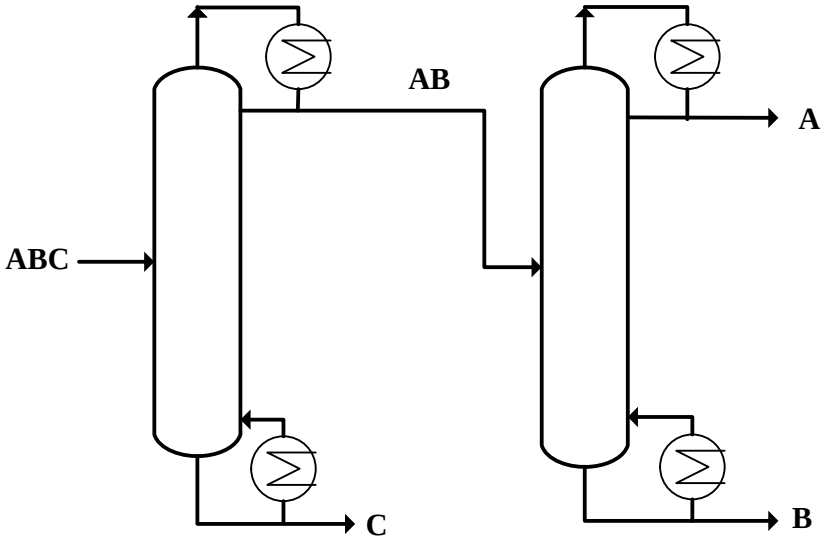


Figure 1-2: Indirect Distillation Column Sequence

1.2.3 Distributed Column Sequence

This sequence needs three distillation columns for the required separation and contains total six heat exchangers for heating and cooling process. Due to extra number of column and extra heat exchangers, this arrangement requires high investment cost. This arrangement is often used when the separating components has close boiling points and the ternary mixture separation has to be carried out at lower temperature by using low quality utility. This configuration would also be applicable where the feed has higher concentration of middle key component. The distillate stream of 1st column is fed to 2nd column for separation of light and middle key component, and bottom stream of 1st column is fed to 3rd column to separate middle key component from the heaviest component (Figure 1-3).

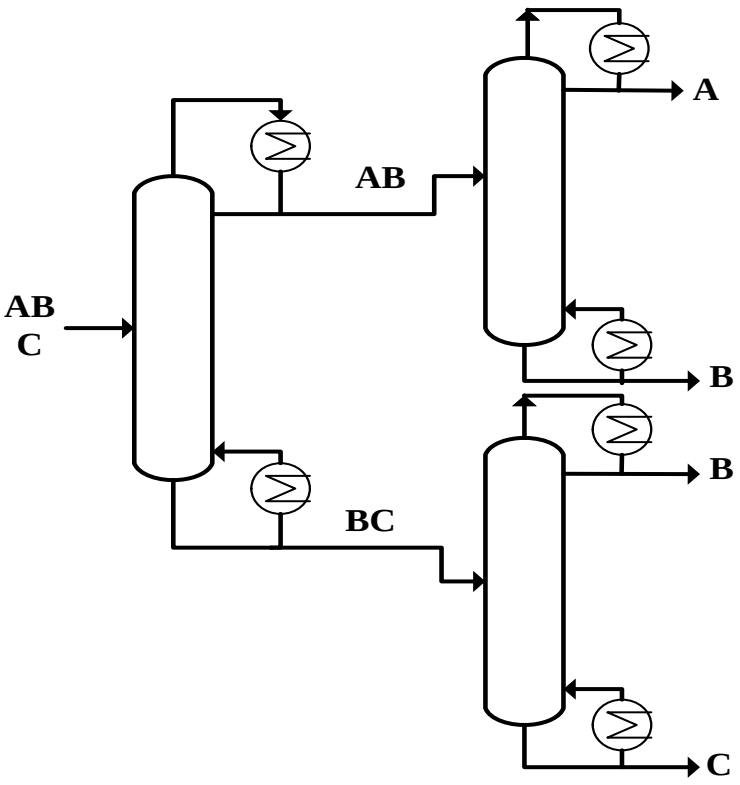


Figure 1-3: Distributed Distillation Column Sequence

This sequence is useful for low temperature processes and for the processes when the relative volatility difference of light, middle and heavy key components is small. This column arrangement has the highest separation efficiency when the partial condenser is used on the first column of the sequence [5]. This column configuration divides the cooling and heating load to intermediate reboiler and condenser of the first column in the sequence.

1.2.4 Remixing Effect in Conventional Distillation Columns

The main drawback with the use of simple column configuration is its thermal inefficiency. This thermal inefficiency in these conventional distillation arrangements is due to remixing effect. Schultz et al [6] discussed this thermal inefficiency in detail. For direct distillation column sequence, concentration profile for middle boiling component B in 1st column is shown in Figure 1-4 [6].

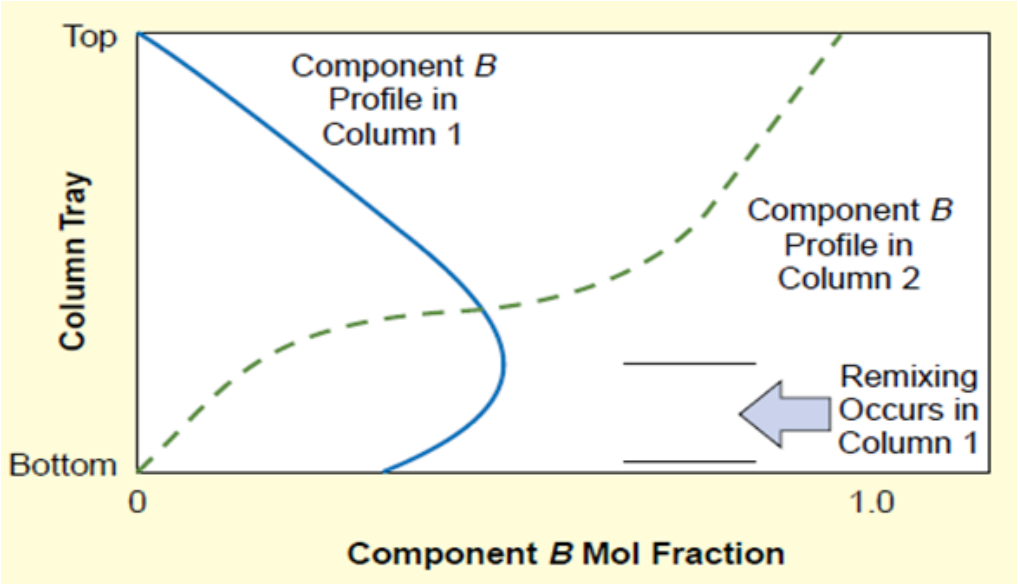


Figure 1-4: Remixing Problem of Middle Component in Direct Column Configuration [6]

It can be seen that in 1st column, the middle boiling component B concentration reaches to maximal purity at some tray location near the bottom tray. Below this tray, the heavy component C concentration continues to rise and diluting B in such a way that its

concentration profile continues to decrease for each tray while proceeding towards the bottom. Then the component B is not separated in the first column and its starts to dilute due to rise in composition of component C. This dilution phenomena and mixing of middle component with heavy component leads this column arrangement to thermally inefficient.

1.3 Complex Column Arrangements

Complex distillation column arrangements consist of thermally coupled system, heat integration, etc. Thermally coupled system uses two way vapor-liquid connection for heat transfer among the pre-fractionator and the main column. These complex system include side rectifier, side stripper, Petlyuk column, and divided wall column [7].

Simple distillation column arrangements are inefficient due to the irreversible mixing of the non-similar streams. Often, the concentration of middle product goes to maximum value on the intermediary trays and then suddenly decrease to fulfil the overall mass balance. This remixing of the streams is the main source of the separation inefficiency in simple distillation column. By using complex column arrangement, these mixing losses as well as consumption of energy could be reduced. The amount of energy consumption could be decreased by introducing the thermal coupling arrangement between various sections of columns. This thermal coupling can use additional portions (side strippers, side rectifiers, .e.g.) to reduce the remixing of the separating components and reduces the column duties. Pre-fractionator arrangement also reduces the mixing losses that occurs at the feed-tray due to composition difference in the incoming feed liquid and the liquid present on the feed tray. While using thermal coupling arrangement, there is no need of reboiler (side rectifier

configuration), or the condenser (side stripper configuration), or both (pre-fractionator arrangement) due to the direct contact of vapor and liquid between the two columns.

1.3.1 Side Stripper and Side Rectifier Arrangement

In these complex column arrangements, one side (liquid) stream is taken from below or above the feed stage of main column. The required purity of the product could be improved by stripping out light component in side stripper or rectifying heavy component in side rectifier, they are used in refinery distillation and in cryogenic air separation respectively. In side rectifier arrangement, the rectifier is thermally linked with main column and similarly in side stripper arrangement, stripper is thermally linked with the main column. The side rectifier and side strippers are also known as partially thermally coupled distillation system (PTCDS) due to the vapor/liquid connection between the two columns.

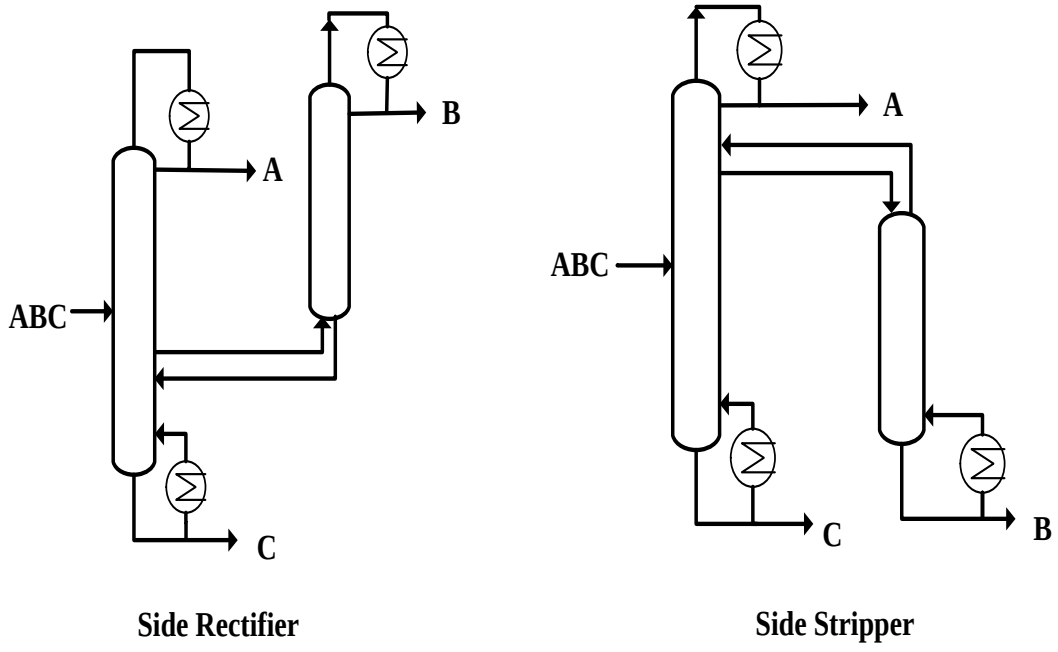


Figure 1-5: Partially Thermally Coupled Distillation Column Schemes

The side stripper do not have one condenser and similarly side rectifier (Figure 1-5) do not have one reboiler as compare to the simple distillation column arrangement.

1.3.2 Pre-fractionator Column Arrangement

Pre-fractionator arrangement splits the feed stream into two streams in first column (pre-fractionator) and then fed to the main column that has also a side draw as well (Figure 1-6). This sequence has some similarity to the distributed column sequence, this sequence could be thought of as distributed column configuration from where some reboilers and condensers are eliminated.

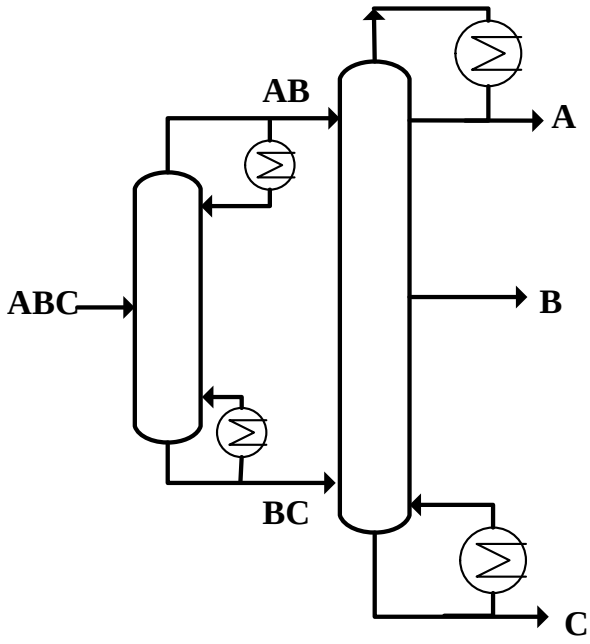


Figure 1-6: Pre-Fractionator Column Sequence

This column sequence is applicable if the ternary feed mixture contains large amount of middle key component. This strategy can also be used for the case when the splits between

all the fractions in the feed are difficult. In order to take benefit of the available utilities at various temperatures, both distillation column should be operate at different pressure.

1.3.3 Petlyuk Column or Fully Thermally Coupled Distillation Column System

This fully thermally coupled distillation column (FTCDC) is also famous as Petlyuk column and has obtained increased acceptance in industries, although its idea was developed 50 years ago [8]. This column arrangement provides additional thermal linking between the pre-fractionator (first column) and the main column (second column) to improve the separation efficiency. Petlyuk column in Figure 1-7 represents a configuration that can separate more than two components by using only single condenser and reboiler.

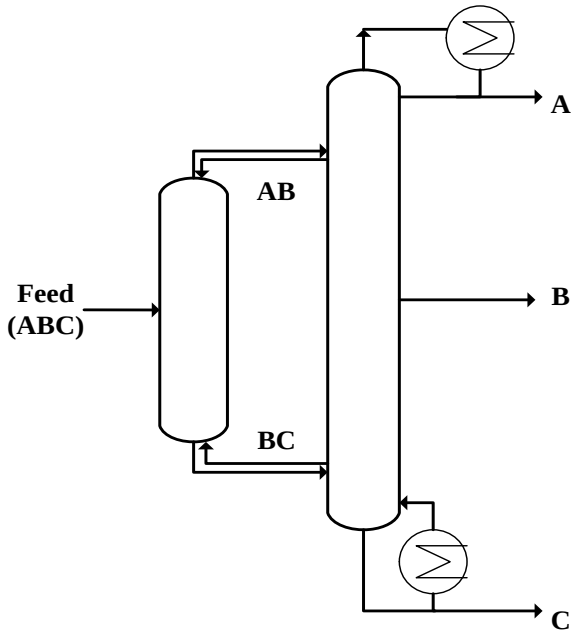


Figure 1-7: Petlyuk Distillation Column (FTCDC)

This column is known as Petlyuk column after presenting the comprehensive study that was done by Petlyuk et al. [9]. This Petlyuk column eliminates the reboiler and condenser

of the pre-fractionator with liquid/vapor interconnection between the two columns. Pre-fractionator of Petlyuk column make a sharp split between light and heavy boiling key components, and intermediate boiling component is naturally distributed among the bottom and top products. Petlyuk column arrangement has greater thermal coupling as compared to pre-fractionator arrangement and this thermal coupling of petlyuk column reduces the separation losses and increase the thermal efficiency.

According to Christiansen et al. [10], Petlyuk column is generally "a column that is capable of separating multicomponent feed mixture by using only one condenser and one reboiler, where any required product purity could be achieved by increasing trays, as long as the separation is feasible thermodynamically." Amongst all the possible alternatives for a three-product distillation column system, the Petlyuk column demands the least amount of rectifying liquid and stripping vapor.

There are more internal flows between the two columns with no hold ups because there is no any intermediate reboiler and condenser. In Petlyuk column, main reason of energy efficiency is the elimination of mixing of feed with liquid on feed tray and remixing of internal streams [11]. The Petlyuk column arrangement contains more operation and design degrees of freedom as opposed to conventional distillation system. This higher number of degrees of freedom causes a complexities in the Petlyuk column design and control [11].

1.3.4 Divided Wall Column

Concept of fully thermally coupled column system was further extended into all in one column concept, which results the emergence of divided wall column. The DWC is basically a Petlyuk column in which the pre-fractionator is located inside a single column

shell along with a dividing wall between the feed side and the side draw section. The key advantages of the DWC are reduction in energy requirement and capital investment savings.

1.4 Three Products Divided Wall Column Structure

Divided wall column for distillation is the most compact configuration. Meeting the growing energy demand and reducing green-house gas emissions to meet the environmental compliances seek more efficient operation and design of the distillation columns. Therefore, DWC has gained increasing application in industry because of its lower energy consumption and capital cost. The DWC offers capital and energy savings. It is only due to fact that DWC has reduced number of equipment (single column shell, single condenser, single reboiler, and less piping etc.) as opposed to the conventional distillation column arrangements [12][13]. In addition the reduced equipment and piping also saves significant space.

The reported capital cost and energy savings related to three product divided wall column is approximately 30%. In DWC, the pre-fractionation section and main column of Petlyuk column are combined into a single column shell and the entire separation task of ternary feed system into its pure components occurs only in one thermally coupled column shell. The DWC structure contains a vertical partition wall inside a column shell to house a pre-fractionator in the same column [14][15]. The vertical partition among the feed side and side-draw section of the column allows more separation efficiency and more capacity. The DWC arrangement is basically for separation of more than two components, for which conventionally two columns were required.

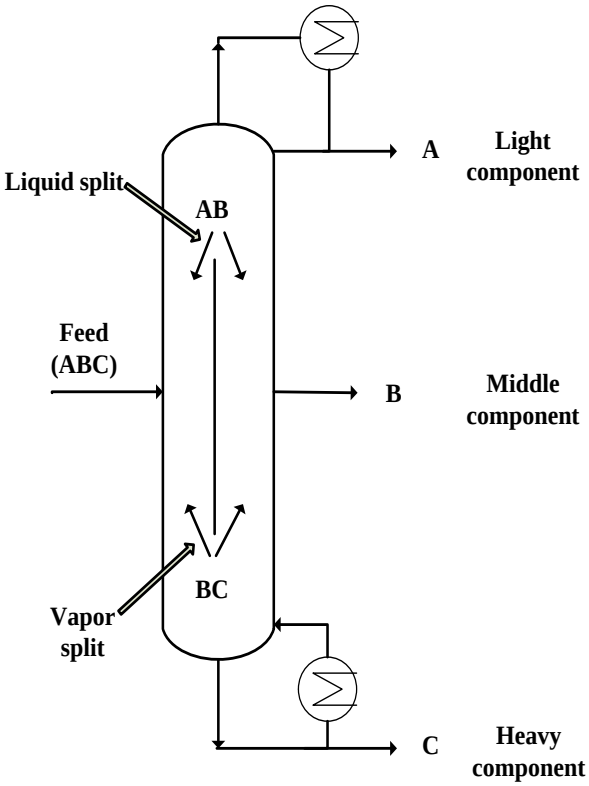


Figure 1-8: Three Products Divided Wall Column

The DWC structure is thermally equal to Petlyuk column (FTCDC) provided the heat transfer through divided wall of column is negligible [12]. The structural diagram of DWC is presented in Figure 1-8. The purity of side product (middle product) from a DWC is greater as compare to the purity obtained from conventional side product column. So whenever highly pure middle product is required, DWC should be used because DWC accomplish the required separation task in single distillation column by using lower amount of energy as compared to simple side draw setup [6].

Different studies shows that DWC structure can save about 30% of energy cost as opposed to the conventional distillation schemes. Despite the high economic benefits of DWC, a lack of knowledge in suitable design method and operation has prevented its wide commercial application. The main reason for the limited use of DWC on industrial scale is

the difficulty in both the operation and control of the DWC. The number of degrees of freedom for the DWC are greater than the conventional distillation column and therefore it is difficult to design and control. The DWC was first time used in 1985 by BASF SE in Germany [16] and at present there are about 70 operational divided wall column in operation by BASF worldwide. The DWC applications have increased rapidly to more than 100 in 2010 [17].

1.5 DWC Configurations

Two different types of DWC configuration could be used for ternary mixture separation. The first type of configuration is shown in Figure 1-9 (a) which is patented by Wright in 1949, and it is the mostly used configuration. In this configuration, the dividing wall as well as side draws and feed is placed near to the center of the column [18].

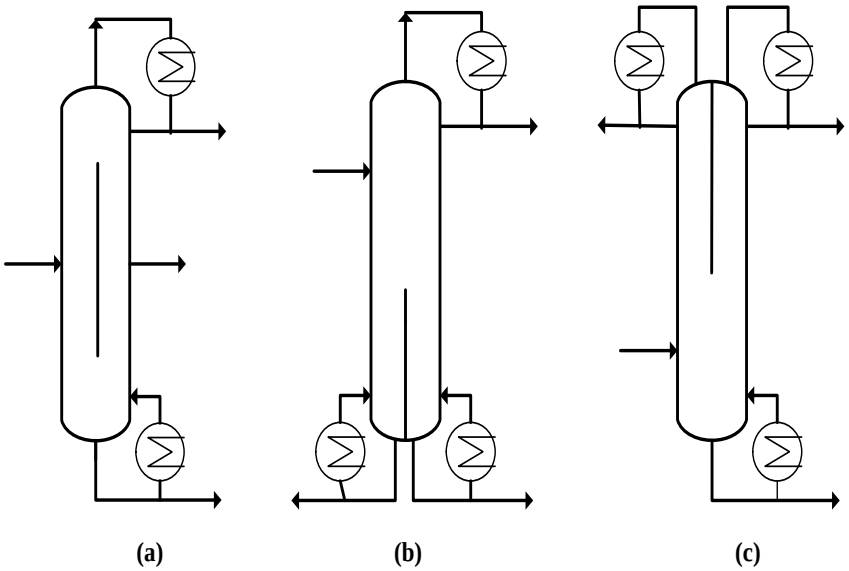


Figure 1-9: Different DWC Configurations [18]

The other type of configuration is shown in Figure 1-9 (b) and 1-9 (c). In this configuration, the dividing wall is positioned either at upper end or at lower end of column. This type of

column arrangement was first time patented by Monro [19] and then utilized firstly in 2004 [20].

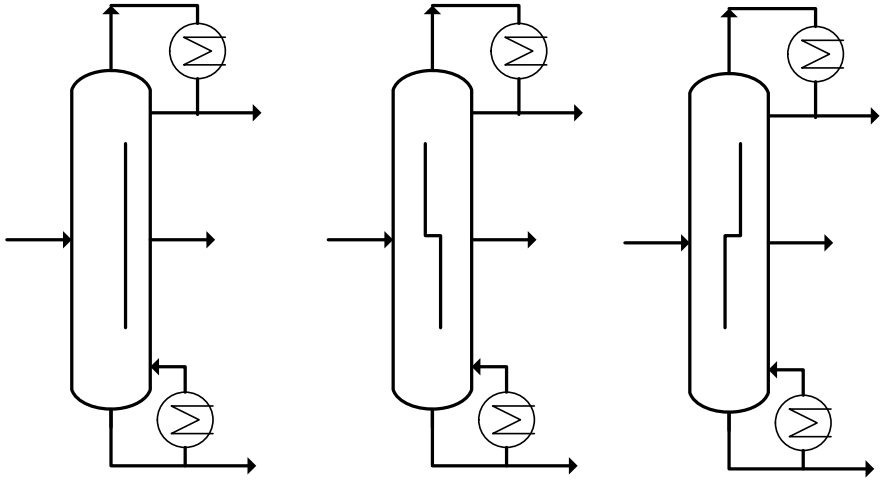


Figure 1-10: Different Shape and Position of Dividing Wall [18]

DWC in Figure 1-9 (b) is known as split column shell with divided bottom sector and joint overhead sector, whereas the DWC in Figure 1-9 (c) is to be known as split column shell with joint bottom sector and dividing overhead sector [21]. Moreover, the wall could be relocated from the center towards the walls of the column as shown in Figure 1-10 (a), and the DWC could have the diagonal sections as well as shown in Figure 1-10 (b) and 1-10 (c).

In the DWC, the required product purity, energy and material balance efficiency depends on the proper selection of the column internals. The DWC could be consists of different kinds of packing or the trays. Generally, it is easy to build a DWC with trays and the welded wall could provide stability to the shell. It is more difficult to construct a packed DWC because it is very complex to welding the wall. During the fitting of packed DWC, one important thing is that the column packing should not be touch with column wall surface

otherwise it results in massive liquid flow and reduces the fractionation efficiency [20]. DWC technology of non-welded wall has been established recently by BASF (Baden Aniline and Soda Factory). The DWC design becomes simpler by using unfixed dividing walls and another benefit of non-welded partition wall is a more accurate and faster installation. Other advantages are less weight and fewer manholes and the revamping of conventional simple distillation column becomes simpler, cheaper and faster [22].

1.6 Advantages of Divided Wall Column

Use of divided wall column has many advantages as opposed to the conventional distillation sequences, where two columns are required to achieve the desired high purity products; DWC has only one overhead condenser and one reboiler. Main attractive advantages that could be obtained using DWC instead of conventional distillation system are the following:

a. Energy saving upto 40% as compared to conventional column.
b. Investment cost saving by minimizing the number of equipment's (less reboiler and condenser).
c. 30-40% smaller plot area than the conventional column and less piping and electrical lines.
d. Uniform distribution of liquid on the trays.

Use of the DWC provides compactness at chemical plants and results in better product qualities. By using DWC, thermal stress for temperature sensitive products can be lowered because product is reboiled only once [18]. The remixing problem of the medium boiling components in the pre-fractionator column can be avoided by the use of DWC. Because of

this reduced remixing effect, the DWC has significantly high thermodynamic efficiency compared to the conventional distillation column. This remixing of medium boiling components in conventional column system cannot be avoided when feed contains more than two components and this remixing is a main cause of thermal inefficiency in conventional column system for the separation of three products [12].

One more significant advantage of DWC is the simple implementation in the revamp projects. The existing conventional distillation column can be retrofit to a DWC by changing only the internal structure of the existing column. Retrofit in the industries is the modification of the existing plant equipment with the new available technologies without any change in the capacity and the major investment. There are two possible revamp options as given below.

1.6.1 Modification of Existing Column Internals without Replacement of Column Shell

In this option only the relevant part of the existing column is modified where the partition wall is to be installed. The internals along with trays and support rings are uninstalled in the dedicated portion. Then the dividing wall is installed in required segments through the manholes in a proprietary method. In the end, the new internals, trays along with all devices are installed.

1.6.2 Modification of Existing Column Internals with Replacement of Partial Column Shell

This method is very attractive for smaller diameter column. Part of the column shell where the dividing wall is to be installed is replaced by a new section. The new column section

where the dividing wall is installed is prefabricated and latter welded to the remaining bottom and top column parts [23].

1.7 Industrial Applications of Divided Wall Columns

Now a days divided wall columns are used for multicomponent mixture separation. Initially, applications of DWC were set up for the systems having small fractions of heavy and light key components. Now DWCs are being used to produce high purity grades and used for the fractionation of various systems, for example hydrocarbons, aldehydes, alcohols, acetals, ketones, amines, etc. Additionally, DWC could also be used in reactive, extractive and azeotropic distillation. Industrial applications of DWC system stated in published literature are given in Table 1-1 [1]. Most of them are used for the separation of ternary system. Table 1-2 lists a number of different available industrial applications for three component system [1].

Table 1-1: Industrial Applications of DWC Stated in Literature [1]

Industrial Examples	No. of Columns
Ternary system	117
Multicomponent system	4
Reactive distillation system	-
Azeotropic distillation system	1
Extractive distillation system	3
DWC renovations	4

Table 1-2: DWCs Applications for Ternary Mixture Systems [1]

Organization	Process system	Constructing company	Description	References
1. Sasol, Johannesburg South Africa	Hydrocarbons separation from Fischer-Tropsch synthesis unit	Linde AG in 1999	-World's largest DWC -Height 107 m -Diameter 5 m	Schultz et al. (2002) Parkinson (2005)
2. Veba Oel Ag, Germany	Separation of benzene from pyrolysis of gasoline	Uhde in 1999	-170000 mt yr^{-1} feed capacity	Schultz et al. (2002) Yildirim et al. (2011)
3. Saudi Chevron Petrochemicals Saudi Arabia	Undisclosed	Uhde in 2000	-140000 mt yr^{-1} feed capacity	Yildirim et al. (2011)
4. Lonza, Visp, Switzerland	Separation of various ternary mixture	Undisclosed	-Height 10 m -Diameter 0.5 m	Grutzner et al.(2012)
5. Exxon Mobil, Rotterdam Netherlands	BTX fractionation	Exxon Mobile 2008	-No data available	Parkinson (2007)
6. BASF SE, various sites	Mostly undisclosed	Most column built by Montz GmbH	- 70 DWCs -Diameter 0.5-4 m -Operating pressure	Amminudin et al. (2001) Olujic et al. (2009) Kaibel et al.(2004)
7. Undisclosed	Separation of aromatics from paraffin	UOP	-Five DWC -Trap tray	Schultz et al. (2002, 2006)

1.8 Motivation

One of the main focus of today worlds is the reduction of CO2 emissions that has been increased significantly in recent years [24]. All industries are the main source of these large amount of emissions, therefore any minor savings in energy could results in less CO_2 emissions. Distillation alone accounts for the major portion of the energy consumption in process industries. To come across the growing energy demand and to reduce the green-house gas emissions for the environmental compliance, there is a need of efficient design of distillation column.

In current scenario of industry competition, DWC is a best attraction for process industries to reduce energy consumption to about 35% than the conventional distillation system. The DWC has been implemented successfully in some industries and it has gained increasing applications due to its attractive advantages, which is the major motivation of this research topic. Due to current economic collapses and successive boom in the market, industries are insecure and they are careful in taking decision while go for a new plant. An alternate way is to operate the plant more effectively and efficiently by making some modification in the existing plant equipment's [25].

There is very limited published literature available on the optimal design method of the DWC, which is the motivation for the research that is presented in this study.

1.9 Research Objectives

The following are the objectives of present study.

1. Design the conventional two-column distillation system and compute the energy consumption required to carry out the given separation task.
2. Design and optimize the three products DWC and find the optimal design parameters.
3. Develop the detailed guidelines of economic evaluation of DWC for a given separation task.
4. Find economical design of the DWC based on minimum total annual cost.

CHAPTER 2

LITERATURE REVIEW

Before proceeding to further study, it is very compulsory to understand the history of the divided wall column and conventional distillation column configurations. Literature review forms an important part of research which helps to initiate the study with some important information from the past research activities globally. The extensive literature review exhibits that the DWC for distillation is currently receiving positive response from industry because of its energy saving capability and reduction in capital cost. This significant reduction in energy consumption for distillation process has motivated many researchers to develop various distillation column configurations that could carry further savings in consumption of energy and investment cost. Fully thermally coupled distillation system concept was extended into all-in-one concept, which marks the emergence of DWC. Therefore the literature related to fully thermally coupled distillation column is also included in present literature survey.

2.1 Background

The concept of fully thermally coupled distillation column which is famous as Petlyuk distillation column is established 50 years ago. Remarkably, this Petlyuk column is not limited to separation of only ternary mixtures. According to Skogestad et al. [10], FTCDC or Petlyuk column is generally, "column configuration, separating more than two components by using single condenser and single reboiler, where any required purity level could be achieved by increasing column trays, if separation is thermodynamically

feasible". The DWC idea with thermal coupling was first time introduced in 1930s [19] and 1940s [26][14]. The conventional direct column sequence, indirect column and distributed column sequence evolved to fully thermally coupled distillation arrangement [27], the Petlyuk column comprises of two thermally coupled columns. Petlyuk et al. [9] also presented thermal coupling for ternary mixture separations. The evolution of the DWC and FTCDS comes from the energy demand and capital cost saving. Use of DWC enables at least two conventional column arrangements to be replaced by a single column. More than two separations could be performed in a single column by using direct coupling of heat flows. In DWC, mixing losses can be minimized by heating the feed on one side of the dividing wall [28].

Kaibel [15] reveals that BASF AG is the first company who applies the divided wall column commercially and then have successfully commissioned. All over the world, about 100 divided wall column are operated and among these columns 30 are operated in the BASF group. This study shows the increasing trend in the number of columns by BASF (Baden Aniline and Soda Factory) and ensures the acceptance of DWC technology.

In available literature, fully thermally coupled distillation system has been considered as special arrangement due to its thermal efficiency. Fidkowski et al. [29] concluded that Petlyuk column demands minimum amount of rectifying liquid or stripping vapor for its operation as compared to the other distillation column sequences and this minimum amount of vapor flow is also applicable for DWC. Due to this lower vapor flow rate in the DWC, the heat inputs requirements of condenser and reboiler are less. Regardless of the high prospective of DWC economic edge, a lack of suitable structural design method and complexity in control has prevented commercial use of DWC. Triantafyllou and Smith [30]

concluded that by using Petlyuk column about 30% energy saving can be accomplished in replacement of conventional two-column configurations.

2.2 Different Design Studies of DWC

Design structure and optimization of DWC has been investigated in available literature. Most of the researchers used fundamental mathematical equations as a part of shortcut design method to get the initial design followed by rigorous simulation.

The initial work was done by Underwood (1948) who used a rigorous iterative method. This method was based on material balance equations. Further Petlyuk has taken a step and published a series of research papers on thermodynamically optimal distillation arrangement. Their proposed method has laid the foundation and can be used as guidelines while trying to analyze the original distillation columns.

Fidkowski et al. [31] studied the FTCDC at minimum reflux ratio, but structure of their designed column was not considered. Their study results were very interesting for the design of Petlyuk column. They found the design parameters required for optimal Petlyuk column operation analytically by assuming constant relative volatility and ideal mixture. Triantafyllou and Smith [30] suggested a shortcut design technique to design and optimize the FTCDC by using three column arrangements. They used shortcut design method for each column to get reliable initial estimates required for rigorous simulation. In their research, they presented simple optimization approach by taking into account both minimum energy cost (reboiler duty) and capital cost instead of employing minimum vapor flow criteria. The shortcut method was further validated by using rigorous simulation on process simulator. They identified many design parameters that are required to be

optimized. They did not mentioned the rigorous simulation procedure for the designing of FTCDC by using process simulator. Finally, they concluded that acceptance of DWC technology will bring significant savings in capital cost along with all the savings realized by Petlyuk column. Mizsey et al. [32] theoretically studied the design of the divided wall column and reported 30% saving in energy cost as well as capital cost due to operation of DWC as compared to conventional two binary distillation column for ternary mixture separation. Agrawal et al. [33] studied the design of FTCDC and modified it by excluding one connection between the main column and the pre-fractionator. Dunnebier et al. [34] developed optimal design method for DWC with minimum capital and operating cost, design was based on mathematical programming and massive calculations as compared to shortcut design method.

Abdul Mutalib et al. [35] reported, it is very unfeasible to operate vapor split in DWC structure but liquid split can be regulated easily by using specially designed liquid distributor. On the basis of results for their simulation studies, they reported that DWC could be operated effectively. Agrawal et al. [36] proposed fully thermally coupled arrangement by removing one or two of four interlinking streams between the columns and introduced the design without any inter-column vapor transfer. Rong et al. [37] studied the thermally coupled distillation columns and showed that column configurations with side rectifiers and side strippers could offer attractive benefits for separation of multicomponent mixture as compared to conventional column sequences.

Amminudin et al. [38] presented semi-rigorous model for initial design structure and optimization of FTCDC that was based on equilibrium stage composition concept. They use component composition to find out all the design variables in each column section. In

their research, they divided FTCDC in two different sections to remove the interconnection in streams and obtained the optimal design which was further confirmed by rigorous simulation. However, it was a lengthy process to optimize the whole design parameters to obtain the optimized design structure. Hernandez et al. [39] suggested the procedure to design the thermally coupled column by explaining the control system of thermally coupled distillation system.

Kim [40] developed a design method for fully thermally coupled fractionation column, structural design method of FTCDC was proposed on the basis of the liquid composition calculations where the actual tray number was set to twice the minimum tray number. Caballero et al. [41] presented the synthesis of distillation arrangements for separating non-azeotropic feed mixtures into their product streams. The proposed design method considered both thermally coupled system and conventional column system in the same design model. They showed that for the sharp separation of multicomponent mixture, it is possible to build up a design structure that considers all the possible options, from thermally coupled arrangement with single condenser and reboiler to arrangement with conventional column arrangements.

Kolbe et al. [42] studied pyrolysis gasoline fractionation for benzene recovery by using DWC. They concluded that by using DWC the remixing effect of medium boiling component in pre-fractionator can be avoided and high purity of side stream can be obtained. Finally, they showed the following considerable savings obtained by using DWC fractionation as compared to conventional column sequence: 35% in operating energy cost, 25% in capital cost and 40% in plot space. DWC offers less space requirement due to less number of condensers, reboilers and associated equipment's.

Kim [43] proposed a rigorous design method for FTCDC. In his study, the proposed structural design eliminated the tedious iterative computation which was encountered in the conventional column design procedures. He observed that when concentration of middle key component in column is prominent, number of stages in pre-fractionator was near to stages number in middle-portion of main column. He claimed that the mixing in feed tray lowers the column thermodynamic efficiency more than the remixing of middle boiling component. Therefore a separate pre-fractionator is better than DWC structure unless the composition of middle boiling component in feed and side product is close. Blancarte et al. [44] established a design method for structural designing of thermally coupled system such as side stripper and side rectifier followed by thermally coupled column system.

Muralikrishna et al. [45] proposed the design of conventional column configuration based on Fenske-Underwood-Gilliland correlations. They extended these correlations to design the DWC by dividing the DWC in three columns. He represented the design variables of DWC graphically in a 3-dimensional plot. The proposed design model was further confirmed by rigorous simulation in process simulator. Jimenez et al. [46] studied the design structure and energy performance of fully thermally coupled column using simulator. In their study, they did not provide the simulation procedure for separation of multicomponent mixture. Lee et al. [47] designed and optimized the fully thermally coupled distillation columns by using process simulator and he extended this design method to design the DWC.

Kim et al. [48] suggested a semi-rigorous design model based on the equilibrium stage composition concept. In this design method, design parameters were find out by using the

feed composition, middle product composition and internal liquid flow rates in both columns (pre-fractionator and main column). Adrian et al. [49] studied the structure of divided wall column and concluded that the DWC will give the best economic. Kim [50] developed an innovative structure of FTCDC with a pre-fractionator and post-fractionator to the main column for the column efficiency improvement. Performance evaluation of proposed design structure was done on process simulator and the proposed design method was extended to DWC. He concluded that by tuning the vapor and liquid split ratios, 29% energy saving could be obtained.

Halvorsen et al. [51] developed analytical Underwood methods to determine the operational parameters of Petlyuk column as a function of relative volatilities, feed enthalpy and feed composition. They used this method to determine the theoretical efficiency of Petlyuk column for any feed mixture. They concluded that about 40% energy savings could be obtained when operation of pre-fractionator occurs at its preferred split and composition of feed is adjusted in a way that lower and upper portions of main column operate at minimum reflux condition. Wenzel et al. [52] have proposed a comprehensive technique for the cost optimization of the divided wall column. They used evolutionary algorithm and shortcut method for the optimization of DWC.

Rong et al. [53] presented innovative technique for analysis of thermodynamically equivalent structure (TES) for Petlyuk column system. The new method was consists of solving two main issues for the synthesis of the TESs for Petlyuk column. First, by using mathematical formula they calculated total number of thermodynamically equivalent structures (TES) theoretically. Second, a step-by-step procedure was developed to generate all the possible TESs. Abad-Zarate et al. [54] studied Petlyuk column by using equilibrium

and non-equilibrium stage composition models. In their study, the simulations of Petlyuk column and conventional column sequences were carried out using process simulator for ternary mixture separation. They resulted that both models predict substantial savings in consumption of energy.

Suphanit [55] suggested that the thermal efficiency of the DWC could be enhanced by allowing heat transfer across the dividing wall. Heat transfer effects through divided wall were investigated by taking into account column grand composite curve (CGCC). Noori Sotudeh et al. [56] developed a design procedure for the DWC on the basis of the Underwood equation. The DWC was divided into three column model and the compositions of interlinking streams of pre-fractionator and main column were taken as design variables. They used Underwood's equation to estimate the number of stages of the main column and set the pre-fractionator stages equal to number of stages in middle section of the main column. Fernando et al. [57] studied the design methodology of divided wall columns and this design methodology was founded on optimization techniques named as genetic algorithms that was written in Matlab.

Noori Sotudeh et al. [58] proposed a design method for DWC system with feed mixtures consisting more than three components with sharp separation and constant relative volatilities between the separating key components. They showed that the minimum reflux ratio and optimal number of column trays could be obtained by Underwood's equation. They claimed that this proposed design method could be used for rigorous simulation of DWC with any process. Hernandez [59] studied the fractionation of binary system (water and ethanol) through fermentation process with two thermally coupled extractive distillation arrangements and one simple extractive distillation column. Analysis showed

that fully thermally coupled extractive system could save 30% energy as compared to simple extractive distillation unit. Lee et al. [60] proposed a modification of the column arrangement by splitting the main column in two different columns at a point of side product draw tray with the purpose to enhance the operability of fully thermally coupled column. Grossmann et al. [61] presented improved group methods to design FTCDC with better predictive capabilities for distillation.

Premkumar et al. [62] suggested a design method for the divided wall column. In their proposed design method, initial structure of DWC obtained by shortcut design method was further optimized by a rigorous simulation in process simulator. Cristofer Bravo et al. [63] proposed an optimal design method of the extractive DWC by means of multi-objective optimization method. Results of their study showed that DWC is a feasible alternative for the fractionation of extractive mixtures. Finally they concluded that this optimal design method could be related to higher thermodynamic efficiencies and lower greenhouse gas emissions. Holland et al. [64] proposed the model of the Petlyuk column in which the column was splitted into different sections and profile map of column were developed for each sections by using various mathematical equations.

S. H. Lee et al. [65] proposed an efficient design procedure for the optimal design of DWC. In their research, DWC was sub-divided into four different segments and compared with sloppy configuration of three conventional column configurations. In proposed design structure, the mole fractions of light and heavy keys were taken as design variable for each column. They observed that design structure that allows energy efficiency in shortcut column structure also gives better energy efficiency in divided wall column. But both DWC and sloppy arrangement have different internal liquid/vapor flow distribution.

Hwang et al. [66] proposed a modified fully thermally coupled column by using existing columns of conventional column sequence. Benzene-toluene-xylene separation system was used in design structure of modified distillation column. Performance of proposed design method and control was evaluated by using process simulator. Ghadrdan et al. [67] developed the shortcut design method for Kaibel distillation columns based on minimum energy diagrams and they extended the three products DWC design concept to four products distillation column (Kaibel column). They studied two different objectives and then realized that control of DWC is very complex when it is operating at minimum vapor flow rate and at fixed product purities.

Chu et al. [68] suggested a shortcut design scheme for DWC design. They divided the DWC in five segments and component net flow model was utilized to obtain the mole fractions of the key components in pre-fractionator. Rong [69] studied the DWC structure thoroughly and formulated a technique for the synthesis of DWC from conventional distillation configurations. In this study, he developed a four step method which generated all the possible DWCs from conventional column configurations. He used quaternary distillation process to demonstrate the DWC synthesis procedure that is valid to any feed mixture.

Ramirez-Corona et al. [70] added post-fractionator with Petlyuk column to modify the structure and studied modification effects on Petlyuk column performance. The proposed design approach could approximate the composition of the interlinking streams. Dejanovic et al. [71] developed the comprehensive design method of the DWC using commercial process simulator. They used four-column model for the simulation of three product DWC. They also developed the cost estimation procedure in their proposed design method which

enables the proper evaluation of the industrial feasibility of a DWC equipped with structured packing. Lee et al. [72] utilized the response surface to instantaneously design and optimize the distillation system. They presented a utilization of DWCs for combination of depropanizer and debutanizer in recovery process of natural gas liquids. In their study, optimization of DWC was done by using response surface methodology (RSM). Their study concluded that DWC compactness is cost-effective and could be used in recovery process of liquids.

Deeptanshu Dwivedi et al. [73] studied the design of three-products divided wall column. The objective of their study was to attain required product purities by minimum consumption of energy (V_{min}). Their main focus was on the control scheme selection. Errico et al. [74] studied DWC and considered DWC arrangement for fractionation of four component mixture. In their study, to design the DWC a shortcut method was used to obtain the necessary input parameters that are required to start the rigorous simulation of the DWC. They concluded that effective amount of energy saving was attained with DWC arrangement. Halvorsen et al. [75] proposed idea of V_{min} diagram for energy consumption analysis to separate the components mixture in distillation unit. They presented that V_{min} diagram can be used for DWC design and to initialize simulations. This V_{min} diagram also utilized to check the minimum energy needed for sharp split of components in conventional and fully thermally coupled systems. They also proposed the computation method to construct the Vmin diagram.

Ambari et al. [76] proposed the operation of energy efficient DWC at available energy (vapor flow rate) lower than the minimum energy (Vmin) required for optimal operation of DWC. Sangal et al. [77] presented the simulation study of divided wall column to

determine the energy performance, product quality, vapor split and reflux rate for the fractionation of ternary mixture of paraffin. They used Box-Behnken design for DWC parameters optimization. Hosanna et al. [78] proposed a new structural design procedure combining Kremser group methods and approximate methods for determining optimal design of FTCDC. In their study, analysis of various feed mixtures was done to study the effects of feed composition on structural design performance. The number of trays in pre-fractionator were estimated by using Kremser group methods. Then Fenske's equation was used to determine number of stages in main column.

Kim et al. [79] studied the application of DWC in gas separation process in floating liquefied natural gas plant. They studied the design structure and operational problems of the DWC while its utilization on offshore LNG plant. In their study, depropanizer and debutanizer of LNG plant were replaced with a single column DWC. After comparing the simulation results with those of conventional column system, they concluded that use of the DWC on floating LNG plant has provided compactness to the distillation system. Utilization of the DWC has reduced the investment cost by 12.5%, and reduced the total utility cost by 20% as opposed to the conventional column system.

Uwitonze et al. [80] develop a new design scheme for fully thermally coupled system. This study was carried out on the basis of approximate group method for fully thermally coupled system design. The component net flow model is utilized to estimate the composition of product in each column segment. In this design method, the number of stages for each column segment is measured based on its end product compositions and operating conditions (flow rates). Sangal et al. [81] used Box-Behnken surface statistical design (BBD) based on response surface methodology (RSM) to study the process parametric

optimization of DWC. They used process simulator for rigorous simulation of DWC with different multi-component mixtures and investigated the effect of changes in process variables on energy efficiency and product quality. They concluded that the proposed design method is fast optimization technique for DWC and it is helpful for industries using DWCs, because optimization of DWC needed less simulation runs and it will reduce the time.

Corona et al. [82] developed a design method for DWC. They modeled the DWC system as non-linear problem based on shortcut design method procedure. They concluded that total energy consumption and capital cost of column is directly dependent on concentration of middle boiling component of ternary feed system. Adiche et al. [83] developed a new shortcut technique to design simple and complex distillation column arrangements. They tested their design method with non-ideal azeotropic mixtures and proved that the design technique is efficient as compared to rigorous simulation methods.

Uwitonze et al. [84] designed new method for the structural analysis of FTCDC. Their proposed design method was composed of approximate group method and Fenske equation. The component net flow model wass used for the understanding of separation phenomenon within column system and for obtaining the end product compositions of pre-fractionator. These end product compositions were used to determine the design of pre-fractionator using group method. For the main column design, the Fenske equation is used. Wang et al. [85] studied the energy efficiency of DWC system. They resulted that the energy efficiency of DWC design with finite number of stages mainly dependent on calculated values of liquid and vapor splits. In their study, they claimed that the proposed control structure could handle both the internal disturbances (variations in liquid and vapor

splits) as well as external disturbances (changes in feed conditions). Luyben et al. [86] [87] proposed new control scheme for DWC that controls the required purity level of the three products and that control structure also reduces the energy consumption. The required product purities were obtained by the control of heaviest component composition in the pre-fractionator. Gerit Niggemann et al. [88] presented detailed analysis of DWCs on the basis of the experimental and simulation studies. Their proposed model showed close settlement between simulation and experimental results for product compositions and temperature profiles.

Sigurd Skogestad et al. [89] studied the control structure of DWC. They experimentally demonstrated that vapor split could be utilized effectively as degree of freedom throughout operation of the DWC, Petlyuk and Kaibel column. They concluded that energy requirement for multicomponent feed separation directly depends on the vapor split and optimal operation could be achieved if vapor split is accessible as a degree of freedom.

2.3 Summary

The literature review discussed above shows the emergence, benefits and attractiveness of the DWC. The DWC will get more importance in future due to energy crises and escalation in energy costs. In the above literature, different researchers proposed their design methods and all the design procedures have their own merits and demerits. Because of increased number of design degrees of freedom, still there is no any accurate method for optimum design and optimization of DWC. Therefore, focus of present research is to fill up this gap and to develop an efficient step-by-step method to determine the optimal design of DWC. Furthermore, sufficient information of economic evaluation of DWC and conventional two

column system is also not available. These facts have provided a motivation to focus my research in respective areas.

- Development of shortcut method for the design of DWC the leading to rigorous simulation and optimization for optimal DWC structure.
- Economic evaluation of DWC as compared to the conventional distillation column.

2.4 Research Methodology

2.4.1 Approach of Achieving the Research Objectives

The approach how to achieve the proposed research objectives consists of several steps that are given below:

1. Based upon shortcut method, developed a technique to obtain preliminary design parameters for DWC. The minimum number of trays (N_{min}) are obtained using Fenske equation at total reflux condition, and minimum reflux (R_{min}) for infinite stages number in column is determined by using Underwood equation. The value of actual reflux ratio is chosen as $R = 1.2R_{min}$ in this study.
2. In next step, the preliminary design parameters are used to initiate the rigorous steady state simulation of DWC to obtain nominal design parameters.
3. From the above steps, nominal design parameters are obtained. This DWC design needs to be optimized to get the optimal design parameters. Therefore, the design of DWC is optimized by using optimizing tool in Aspen HYSYS. The range of internal liquid flow rate and internal vapor flow rates are adjusted in optimizing tool and then determined the optimal internal flow rates of liquid and vapor to obtain the optimal DWC structure based on minimum reboiler heat duty.

4. After optimization, the study of the effect of available energy supply (reboiler heat duty) on composition of column products is carried out when distillation column is operated at energy lower than the optimum energy required for DWC smooth operation. The optimum energy needed for column operation is estimated from optimization of DWC.
5. In next step, detailed guidelines of column sizing followed by economic evaluation of DWC is carried out. Economic evaluation is based on minimum energy consumption. The column is sized for both the maximum vapor and liquid load.
6. Further, economic evaluation analysis of DWC with conventional distillation column is carried out. The analysis results in significant difference in energy consumption as well as total annual cost of DWC as opposed to conventional column arrangements.

2.5 DWC Model for Simulation

The standard model for simulation of three products DWC is not available in any commercial software; we have four models to use for the simulation of divided wall column. These models are one-column sequence, two-column sequence with post-fractionator, two-column sequence with pre-fractionator and four-column sequence. In the present study, we will use two-column sequence with pre-fractionator for simulation of DWC or we could implement Petlyuk Column concept as DWC in simulation environment, because Petlyuk column is thermodynamically equivalent to DWC.

CHAPTER 3

DESIGN OF THREE PRODUCT DIVIDED WALL COLUMN

3.1 Design Procedure of DWC

Design of the DWC depends on the selection of column arrangement to represent DWC as well as the modeling approach (design method). At initial steps, it needs describing the column configuration and determination of operating pressure and the thermodynamic model for VLE calculations.

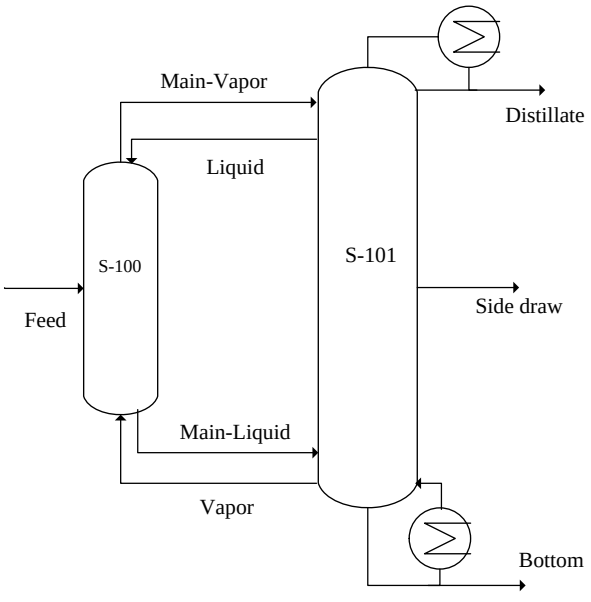


Figure 3-1: DWC Structural Sketch

Figure 3-1 shows the sketch of three product divided wall column along with the parameters that have to be known for the complete design of DWC.

Figure 3-1 shows that feed is entering to pre-fractionator and output streams of pre-fractionator are Main-Vapor and Main-Liquid. Output streams of pre-fractionator forms the feed for main column. The streams Liquid and Vapor are recycled to pre-fractionator. For designing of the DWC, it could be observed that some information is known and remaining have to be assumed for simulation.

3.2 Design Parameters of DWC

The DWC has eight design parameters and all these design parameters have to be determined by choosing some efficient design method. These design parameters are given below.

1. Feed tray location of pre-fractionator.
2. Side product draw stage location.
3. Liquid draw rate.
4. Vapor draw rate.
5. Pre-fractionator trays.
6. Main column trays.
7. Feed stage location of liquid to main column.
8. Feed stage location of Vapor to main column.

3.3 Empirical Rules for DWC Design

There are some empirical rules for designing conventional distillation columns that are also applicable for DWC designing. DWC design parameters needs good initial estimates for simulation convergence. These designing rules are the following.

1. Develop a base case by designing conventional two-column system (Direct column sequence or In-Direct column sequence).
2. The dividing wall could be located in mid third of main column (33-66% H).
3. The DWC total trays could be taken as 0.8 times the total number of trays of conventional distillation system. [$N_{DWC} = 0.8(N_1+N_2)$]
4. The vapor and liquid internal flow rates in DWC could be adjusted as estimated by DWC reboiler duty at 0.7 times the total heat duties of conventional two-column system: $Q_{DWC} = 0.7(Q_1+Q_2)$
5. Equal values of liquid and vapor splits can be used as initial guesses for the simulations.

It is noticeable that these heuristic design rules are enough only to initiate the initial steady-state simulation of the DWC and then a lot of optimization and adjustment in parameters is required to obtain optimal design of DWC based on minimum energy consumption (minimum reboiler duty). Therefore, these rules are not the optimum solution for the design of distillation column [90].

In next section, some design methods are discussed which are used to estimate the design parameters of multicomponent distillation column. These design methods can also be used for the design of three product DWC.

3.4 Different Design Methods of DWC

3.4.1 Shortcut Design Method

Shortcut design method is a fairly rapid design method to measure the initial estimates of the design structure. The initial estimates obtained from the shortcut method are further used to initiate the rigorous simulation using process simulator. Fenske-Underwood-Gilliland method is the combination of the Fenske equation, Underwood equation and the Gilliland correlation. The basic assumptions for shortcut design method are following.

1. Constant relative volatility of the components.
2. Constant molar internal flows.
3. Constant pressure.
4. No internal heat exchange.

In this study, the shortcut method uses Fenske equation, Underwood equation and Gilliland correlation to estimate the required design parameters of the DWC. The procedure to determine these design parameters are given below.

3.4.1.1 Fenske Equation

In 1932, Fenske derived an equation for multicomponent distillation at total reflux. The derived equation assumes that all the stages in column are equilibrium stages. This derived equation was then known as Fenske equation and minimum stages number (Nmin) in column could be estimated by this equation at condition of total reflux. The equation can be expressed as:

$$\left(\frac{x_i}{x_{ref}}\right)_{dist} = \left(\alpha_{i\text{-ref}}\right)^{N_{min}} \left(\frac{x_i}{x_{ref}}\right)_{bot} \tag{3-1}$$

x_i/x_{ref} is the ratio of component i composition to reference component composition. When the fractionation is stated as key components then above equation is rearranged for N_{min} as:

$$N_{min} = \frac{\ln\left[\left(\frac{x_{LK}}{x_{HK}}\right)_{dist} \Big/ \left(\frac{x_{LK}}{x_{HK}}\right)_{bot}\right]}{\ln(\alpha_{LK\text{-}HK})} \tag{3-2}$$

Where α_{LK-HK} is the relative volatility of lighter component to heavier component, x_{HK} and x_{LK} are the compositions of heavy and light key component in the distillation column. Relative volatility can be determined by geometric mean value of component volatility at bottom and top temperatures of the column. Results of Fenske equation could be more accurate for the accurate value of relative volatility. Smith (1963) developed a method in detail to determine relative volatility (α) by calculating geometric average relative volatility and temperatures. Winn (1958) modified the Fenske equation that allows the relative volatility to vary [91]. Both the Fenske and Winn equations are modified by Wankat and Hubert for non-equilibrium stages [92].

3.4.1.2 Underwood Equation

For multicomponent separation system, the minimum reflux ratio could be determined by using Underwood equation. The Underwood equation is

$$\Delta V_F = V_{min} - \overline{V}_{min} = \sum_{i=1}^{C} \frac{\alpha_{i\text{-ref}} Fz_{F,i}}{\alpha_{i\text{-ref}} - \varphi} \tag{3-3}$$

In above equation, feed flow rate is F and component i composition in feed is $z_{F,i}$. If feed thermal condition (q) is known then

$$\Delta V_F = F(1-q) \tag{3-4}$$

Feed thermal condition (q) could be calculated as:

$$q = \frac{Amount\ of\ heat\ required\ to\ vaporize\ 1\ mole\ of\ feed}{molar\ latent\ heat\ of\ feed} \tag{3-5}$$

If feed temperature is given, ΔV_F can be determined by carrying out flash calculation on the feed. $^{\varphi}$ is the root of the Underwood equation. Equation (3.3) is also called the first underwood equation and could be used to determine the appropriate values of $^{\varphi}$. Second Underwood equation is given as

$$V_{\min} = \sum_{i=1}^{C} \frac{\alpha_i \left(Dx_i\right)_{dist}}{\alpha_i - \varphi} \tag{3-6}$$

This second underwood equation could be used to determine the V_{min} and when once V_{min} is known, L_{min} could be calculated from material balance.

$$L_{min} = V_{min} - D \tag{3-7}$$

Similar to Fenske equation, relative volatility could be estimated by average value of volatility at top and bottom temperatures of column. Estimation of bottom and top compositions is needed for relative volatility which could be calculated by using Fenske equation.

3.4.1.3 Gilliland Correlation

Gilliland correlations are developed by Gilliland in 1940. He observed that he could empirically correlates the column stages at condition of finite reflux ratio to minimum reflux ratio ($R_{\min}$) and the minimum stages number($N_{\min}$). After a series of stage-by-stage calculations finally he correlated the function as

$$\frac{N-N_{min}}{N+1} = 0.75 \times \left[1 - \left(\frac{R-R_{min}}{R+1}\right)^{0.5688}\right] \tag{3-8}$$

Where $N_{\min}$ can be calculated by using Fenske equation and $R_{\min}$ by using Underwood equation. Feed tray location could be determined by using relation given below [92].

$$N_F = N.\frac{N_{F,min}}{N_{min}} \tag{3-9}$$

Where $N_{\mathrm{F,min}}$ is the optimum feed plate location at total reflux and it could be estimated by using Fenske equation as.

$$N_{F,min} = \frac{ln\left[\frac{(\frac{X_{LK}}{X_{HK}})_{dist}}{(\frac{Z_{LK}}{Z_{HK}})_F}\right]}{\ln(\alpha_{LK}-\alpha_{HK})} \tag{3-10}$$

In above equation, z_{LK} is the light key composition in feed and z_{HK} is the composition of heavy key. The Gilliland correlations could be used by proceeding as follows:

a) Calculate $N_{\min}$ by using Fenske equation.
b) Calculate $R_{\min}$ [(L/D) $_{\min}$] by using Underwood equation.
c) Select actual reflux ratio (R) which is 1.2 times more than minimum reflux ratio ($R_{\min}$).
d) Determine abscissa.
e) Determine the ordinate value.
f) Calculate actual number of trays (N).

3.4.1.4 Kirkbride Equation

Kirkbride developed an empirical equation to compute the feed stage location in a distillation column.

$$log\left[\frac{N_r}{N_s}\right] = 0.206\log\left[\left(\frac{B}{D}\right)\left(\frac{x_{b,LK}}{x_{d,HK}}\right)^2\left(\frac{x_{f,HK}}{x_{f,LK}}\right)\right] \tag{3-11}$$

In the above equation, N_S and N_r are the stages number in stripping section and rectifying section of column respectively.

3.4.2 V_{min} Diagram Method

Another interesting and effective design approach of multicomponent DWC was proposed by Halvorsen and Skogested. This design method graphically shows the minimum energy (minimum vapor) as a function of distribution of feed. The proposed V_{min} diagram provides a basis to examine the complete flow requirements for complex distillation arrangement in a simple way. This graphical design method mainly based upon Underwood design equation with the assumptions of constant internal molar flows, constant relative volatility of components, and infinite trays of column. The minimum vapor flow (V_{min}) could be determined through Underwood equation and the required input constraints are following.

1. Composition of feed
2. Quality of feed
3. Required product purities (recoveries)
4. K-values

With the known values for all these input parameters, minimum vapor flow (V_{min}) is estimated by Underwood equation and minimum liquid flow that is mandatory to perform separation of a specified multicomponent feed mixture. This design method assumes infinite number of stages which are estimated roughly by considering the stages number equal to four times minimum number of stages ($4N_{min}$) for simulation. This value was proposed by Halvorsen [93] and further assured by rigorous simulations. By using further

thermodynamic models, this V_{min} diagram could also be generated for non-ideal liquid mixtures [94].

This design method describes the vapor and liquid flow required in each segment of the column and column design is based on these internal flows. This design method claims that the lowest energy required to separate feed mixture with n components into high purity products is similar to that needed for the separation of most challenging split. This claim is presented in V_{min} diagram as a highest peak. Initially the stages number is set as two times the minimum stages number which are estimated from Fenske equation. V_{min} diagram is a plot between the vapor flow rates versus overall total flow of column distillate per unit feed (D/F). Enthalpy of the feed is given by the feed thermal condition (q).

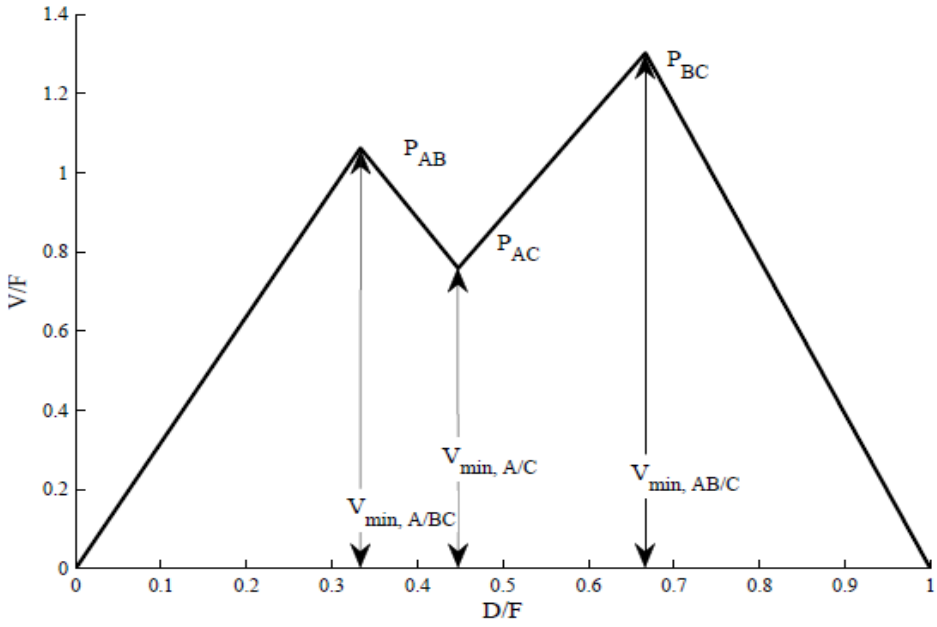


Figure 3-2: Vmin Diagram for Equimolar Ternary Feed System (ABC)

Figure 3-2 represents a plot of V_{min} diagram for an equimolar ternary feed system ABC with liquid feed. In figure, the x-axis represents the net product withdrawal (D/F) and y-axis represents the minimum boil-up rate (V/F) in a simple distillation column. For sharp

separations, the peak point P_{AB} provides the minimum vapor flow (V/F) that is essential for separation of A from BC and the point P_{AC} denotes the minimum vapor flow needed for the separation of A and C, with middle component B distributing to both ends of the distillation column.

CHAPTER 4

SIMULATION STUDIES OF DIVIDED WALL COLUMN

In this chapter, the step-by-step procedure for design and simulation of divided wall column is developed based on shortcut design method using process simulator Aspen HYSYS. The designing of column started with the data available from the plant or from the problem statement such as feed composition, flow rate and temperature, required product purities, column operating conditions and fluid package (thermodynamic model). Thermodynamic model is selected depending upon the separating components.

4.1 Problem Statement

For DWC optimal design, separation task of ternary feed system of ethanol, propanol and butanol has been taken as a case study. This case study has been taken from literature. The characteristics of this case study are given below.

Table 4-1: Feed and Products Characteristics of Case Study

Components	Feed Composition (Mole fraction)	Feed Conditions	Product Specification (Mole %)	Other Conditions
EPB Separation				
Ethanol	0.20	100 kgmol/h	Ethanol: 99%	Column Pressure: 1 bar
Propanol	0.60	1 bar	Propanol: 98.5%	Total Condenser
Butanol	0.20	q=1	Butanol: 99%	NRTL Model

Thermodynamic model predicts the physical properties of the components or vapor liquid equilibrium data for the mixture which is going to be separate. HYSYS also provides some guidance for the selection of proper thermodynamic model for different mixtures. It is very

important to choose the accurate and suitable fluid package (thermodynamic model) for the simulation of DWC, because if the fluid package is not suitable for the given system then there could be simulation convergence problem. To check the feasibility of the selected thermodynamic model in simulation for the given separation task, we could validate the VLE data predicted by the thermodynamic model with the experimental VLE data that is available in literature.

For this alcohol application, the Non Random Two Liquid (NRTL) model which is the extension of Wilson equation is selected for vapor liquid equilibrium calculation that are required in process simulation. The NRTL model uses liquid cell theory and statistical mechanics to describe the liquid structure. This thermodynamic model is also able to represent the physical properties and phase behavior of LLE, VLE and VLLE phase. Similar to the Wilson equation, this NRTL model is consistent thermodynamically and could be used for the ternary or any multiple order system by using parameters retreated from binary equilibrium data.

4.2 DWC Simulation Procedure

Different people proposed different procedures for the design of the DWC. Some of them use graphical design method and some uses analytical design method by applying energy and mass balance on each stage of the distillation column. But the systematic and detailed procedure on how to design DWC using some process simulator is not provided in literature. This chapter provides a detailed step-by-step DWC design procedure using Aspen HYSYS with the data given in the problem statement. In this study the design of DWC consists of the following steps.

1. Shortcut sloppy case (shortcut design method to obtain the initial approximations of parameters needed to perform the rigorous simulation of column).
2. Rigorous sloppy case (rigorous simulation of shortcut sloppy configuration to obtain the internal liquid and vapor flows).
3. Rigorous simulation of DWC
4. Optimization of DWC (optimal vapor and liquid split rate for DWC are found and applied).
5. Economic evaluation of DWC

Rigorous simulation of DWC needs preliminary design parameters for initial design of DWC. These preliminary design parameters are found from the shortcut method calculation that is carried out in process simulator. To obtain the preliminary design parameters of DWC, a three conventional simple column system (sloppy configuration) is selected and it is assumed that it is structurally equivalent to DWC. Sloppy column configuration and DWC configuration are given below.

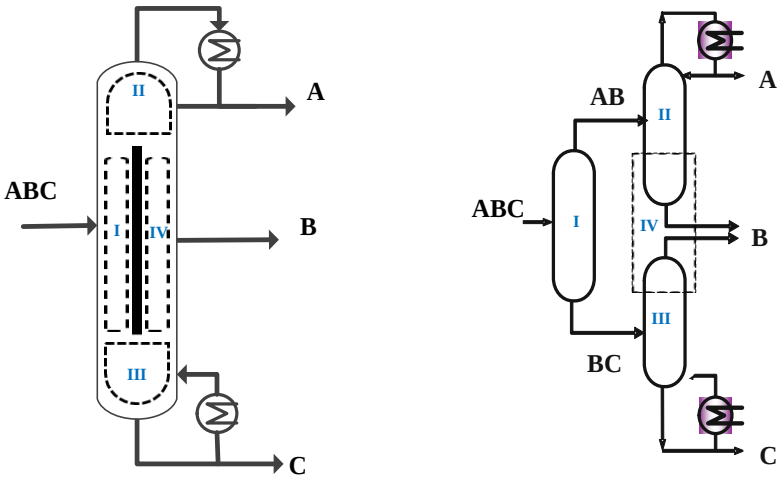


Figure 4-1: DWC and Sloppy Column Configuration

4.3 Shortcut Simulation of Sloppy Configuration (for initial estimates)

The shortcut design method connects the Fenske's equation, Underwood's equation and Gilliland's correlations that relates the actual performance of the column to total and minimum reflux for a given separation. The minimum stages (N_{min}) in a column can be obtained through the use of Fenske's equation, minimum reflux ratio (R_{min}) can be obtained by using Underwood's equation and the actual stages number (N) are found by using the Gilliland's correlation for any reflux ratio (R). The shortcut distillation calculation in process simulator is based on this FUG (Fenske-Underwood-Gillilnad) method where the above mentioned specifications are necessary to complete the simulation and calculation.

To find the preliminary design parameters of the DWC, the three shortcut columns as shown in Figure 4-2 are assumed to be equivalent to divided wall column. This shortcut column model could be used only to determine the initial design parameters of DWC.

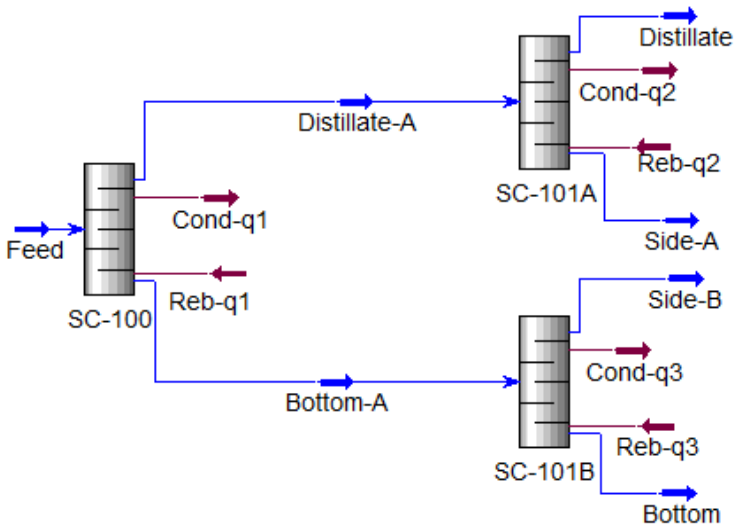


Figure 4-2: Process Flow Sheet of Shortcut Sloppy Configuration for DWC Simulation

The column SC-100 in the shortcut sloppy configuration is assumed to be equivalent of pre-fractionator of the DWC and main column of DWC is equivalent to the columns SC-101A and SC-101B together.

For DWC simulation by using three shortcut columns, open a new case in HYSYS and add the feed components as ethanol, propanol and butanol. Choose the NRTL thermodynamic model as fluid package for vapor liquid equilibrium calculations that are required in simulations. Add the shortcut column SC-100, its material streams and energy streams to the flow sheet as shown in Figure 4-3. Define the feed by the data available in the problem statement. Now open the section "Parameters" and define the required parameters as condenser pressure, reboiler pressure, external reflux ratio, light and heavy key molar purity. The function of column SC-100 is to distribute the middle component propanol to both ends of the column (top and bottom) in a fraction so that most of the ethanol (light component) along with a fraction of propanol (middle component) goes to column top and leave the column as stream Distillate-A. In the same way, butanol (heavy component) and remaining propanol go to bottom of column and leave the column as stream Bottom-A. In the column SC-100 small fraction of light component (ethanol) is present at the bottom along with heavy component (butanol) and small fraction of heavy component is present at the top of the column along with light component. The composition of the heavy key, light key components in bottom and distillate products of 1^{st} column are enetered for the rough initial estimate. Then the pressure of the condenser and reboiler are specified. Adjust the reflux ratio 20% more than minimum reflux ratio (R= 1.2Rm) which is based on heuristics. After specifying all these inputs, the shortcut column SC-100 converges.

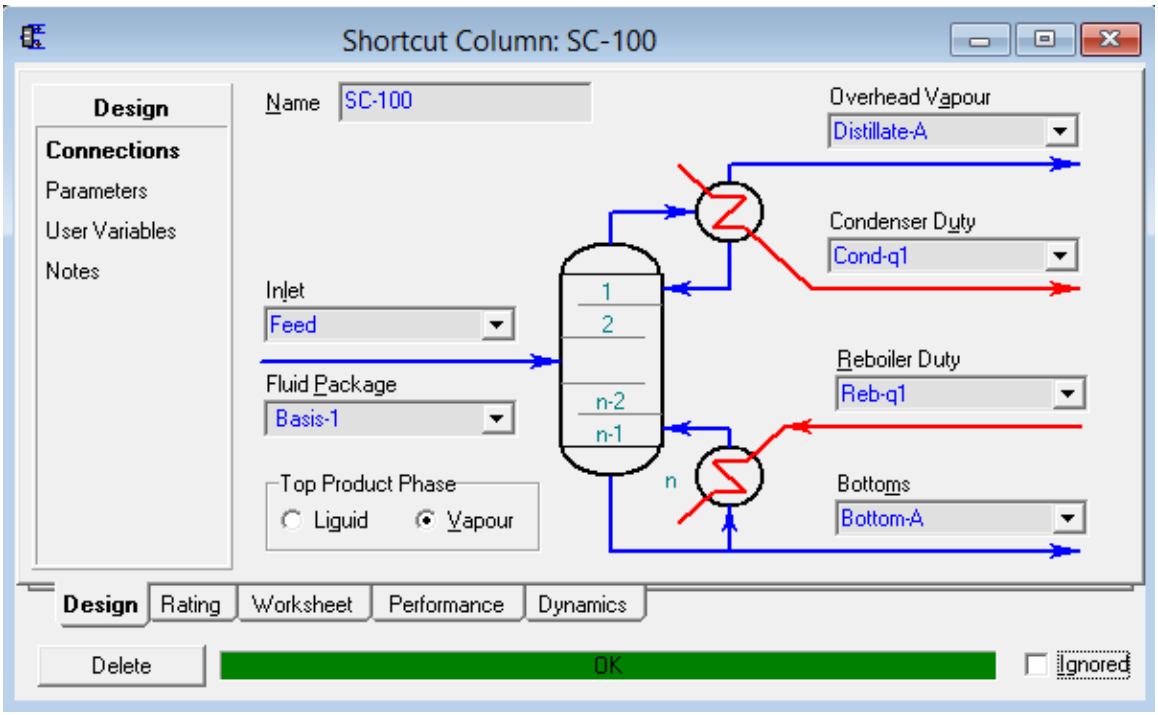


Figure 4-3: Specifications of Material and Energy Streams: 1st Shortcut Column

After converging the column SC-100, another shortcut column SC-101A, its material streams and energy streams will be added to HYSYS flow sheet as shown in Figure 4-4. The function of column SC-101A is to separate the light and middle component (ethanol and propanol). The small fraction of ethanol is present in the bottom of column and small fraction of propanol is present at the top of the column. So, light key in bottom is ethanol and heavy key in distillate is propanol. Since the required product purity of ethanol in the stream Distillate is 99% and the remaining is small fraction of propanol as impurity at the top product of the column. So, propanol fraction in Distillate stream is 1%. After specifying the reboiler pressure, condenser pressure and external reflux ratio, the 2nd shortcut column SC-101A will converge.

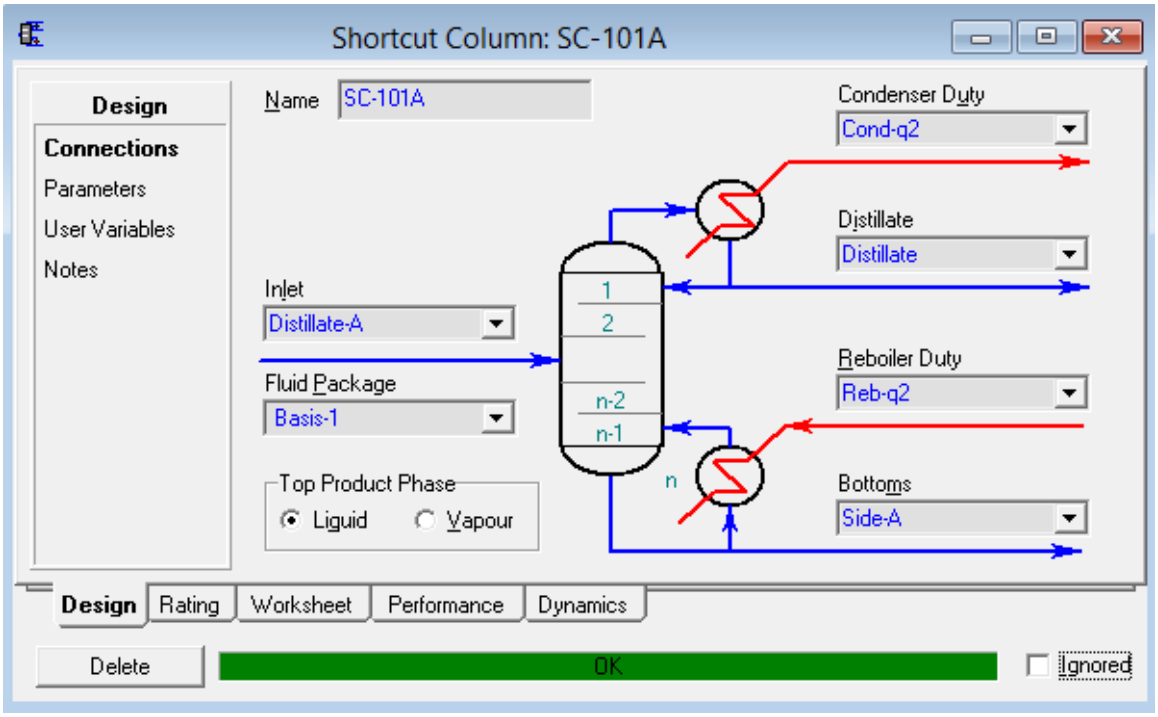


Figure 4-4: Specification of Material and Energy Streams: 2nd Shortcut Column

Similar to previous shortcut columns, another 3rd shortcut column SC-101B, material stream and energy streams are added to the HYSYS flow sheet as shown in Figure 4-5. This shortcut column separates the middle and heavy component (propanol and butanol). The small fraction of propanol is present at the bottom as light key in heavies and small fraction of butanol is present at top as heavy key in lights. The required product purity of butanol in Bottom is 99% and the remaining is the fraction of propanol. Assume that the fraction of butanol that is present at top of column SC-101B is 0.5% as similar to stream Side-A. After specifying the condenser pressure, reboiler pressure and external reflux ratio the 3rd shortcut column SC-101B will converge.

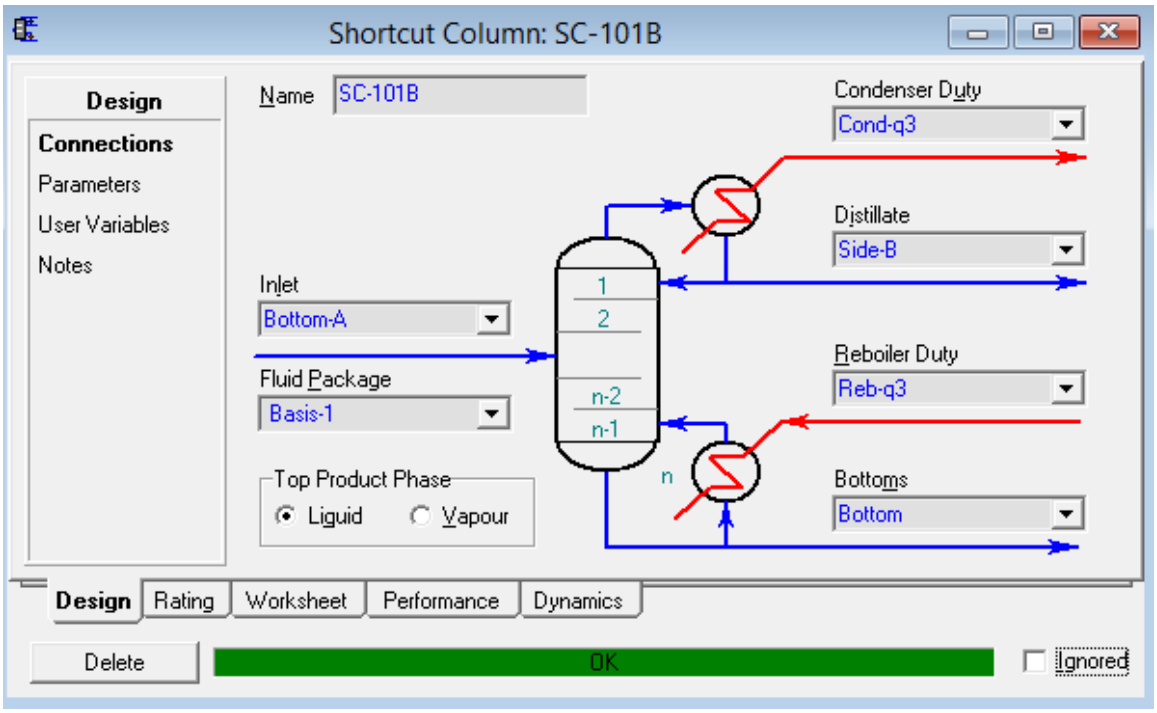


Figure 4-5: Specification of Material and Energy Streams: 3rd shortcut column

After convergence of column SC-101B, the shortcut sloppy configuration will completely converge. The finally converged flow sheet of three shortcut columns (sloppy configuration) is shown in Figure 4-6.

SC-100		
Minimum Reflux	9.805e-002	
Minimum Trays	5.602	
Actual Trays	19.05	
Optimal Feed	10.52	
Condenser Duty	-65.63	kW
Reboiler Duty	627.4	kW

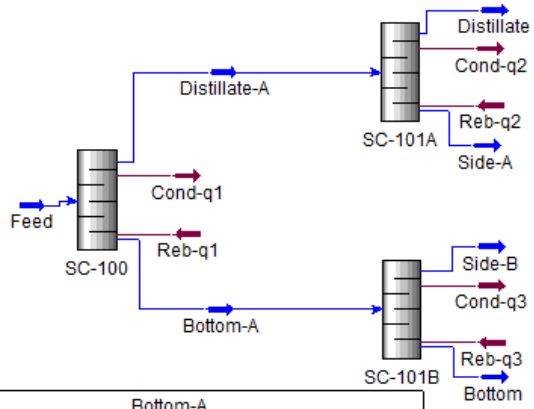
SC-101A		
Minimum Reflux	3.543	
Minimum Trays	12.31	
Actual Trays	26.70	
Optimal Feed	14.06	
Condenser Duty	-1117	kW
Reboiler Duty	574.8	kW

SC-101B		
Minimum Reflux	1.387	
Minimum Trays	13.04	
Actual Trays	30.17	
Optimal Feed	15.75	
Condenser Duty	-994.8	kW
Reboiler Duty	1001	kW

Distillate		
Temperature	72.44	C
Molar Flow	19.61	kgmole/h
Master Comp Mole Frac (Ethanol)	0.9900	
Master Comp Mole Frac (1-Propanol)	0.0100	
Master Comp Mole Frac (1-Butanol)	0.0000	

Side-A		
Temperature	96.65	C
Molar Flow	28.44	kgmole/h
Master Comp Mole Frac (Ethanol)	0.0090	
Master Comp Mole Frac (1-Propanol)	0.9842	
Master Comp Mole Frac (1-Butanol)	0.0068	

Feed		
Temperature	93.95	C
Pressure	100.0	kPa
Molar Flow	100.0	kgmole/h
Master Comp Mole Frac (Ethanol)	0.2000	
Master Comp Mole Frac (1-Propanol)	0.6000	
Master Comp Mole Frac (1-Butanol)	0.2000	



Side-B		
Temperature	96.58	C
Molar Flow	32.11	kgmole/h
Master Comp Mole Frac (Ethanol)	0.0104	
Master Comp Mole Frac (1-Propanol)	0.9846	
Master Comp Mole Frac (1-Butanol)	0.0050	

Distillate-A		
Temperature	87.82	C
Molar Flow	48.05	kgmole/h
Master Comp Mole Frac (Ethanol)	0.4093	
Master Comp Mole Frac (1-Propanol)	0.5867	
Master Comp Mole Frac (1-Butanol)	0.0040	

Bottom-A		
Temperature	105.4	C
Molar Flow	51.95	kgmole/h
Master Comp Mole Frac (Ethanol)	0.0064	
Master Comp Mole Frac (1-Propanol)	0.6123	
Master Comp Mole Frac (1-Butanol)	0.3812	

Bottom		
Temperature	122.4	C
Molar Flow	19.84	kgmole/h
Master Comp Mole Frac (Ethanol)	0.0000	
Master Comp Mole Frac (1-Propanol)	0.0100	
Master Comp Mole Frac (1-Butanol)	0.9900	

Figure 4-6: Flow Sheet of Finally Converged Shortcut Sloppy Configuration: Alcohol Application

Table 4-2: Main Structure of the Shortcut Sloppy Column Configuration: Alcohol Application

	1st column	2nd column	3rd column
Light Key	Ethanol: 0.0065	Ethanol: 0.0090	Propanol: 0.010
Heavy Key	Butanol:0.0040	Propanol: 0.010	Butanol:0.0050
Ext. Reflux Ratio	0.118	4.252	1.664
Total Stage No.	20	27	31
Feed Stage No.	11	15	16
Rectify Vapor (kmol/h)	53.70	102.96	85.55
Rectify Liquid (kmol/h)	5.650	83.354	53.44
Stripping Vapor (kmol/h)	53.70	54.913	85.55
Stripping Liquid (kmol/h)	105.65	83.354	105.39

4.4 Simulation of DWC for Nominal Design Parameters

Once preliminary estimates are completed, then in order to complete the design structure of DWC the simulation is performed by using HYSYS to obtain the nominal design parameters results. This simulation of DWC consists of two steps. In first step, the initial design parameters obtained from shortcut design method in previous section are validated through simulation of sloppy configuration.

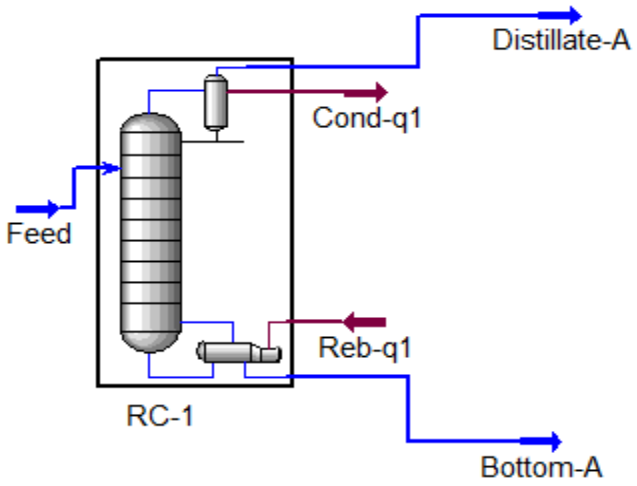


Figure 4-7: Process Flow Diagram of Rigorous Simulation for Column RC-1

For first step, open a new case in HYSYS and add the key components of ternary feed mixture of alcohol. Select NRTL model as fluid package for VLE calculations and enter to the simulation environment. In this simulation environment, add the distillation column RC-1, its material streams Feed, Bottom-A and Distillate-A for column RC-1 as given in Figure 4-7.

Now take the initial estimates from the shortcut calculations. Now connect all necessary streams to the column, define the feed plate location and stages number of column RC-1. The initial approximation of number of stages for RC-1 is obtained from the shortcut calculations which is required to initiate the rigorous simulation of column RC-1. After defining energy streams (Cond-q1 & Reb-q1) the flow sheet will complete as shown in Figure 4-8.

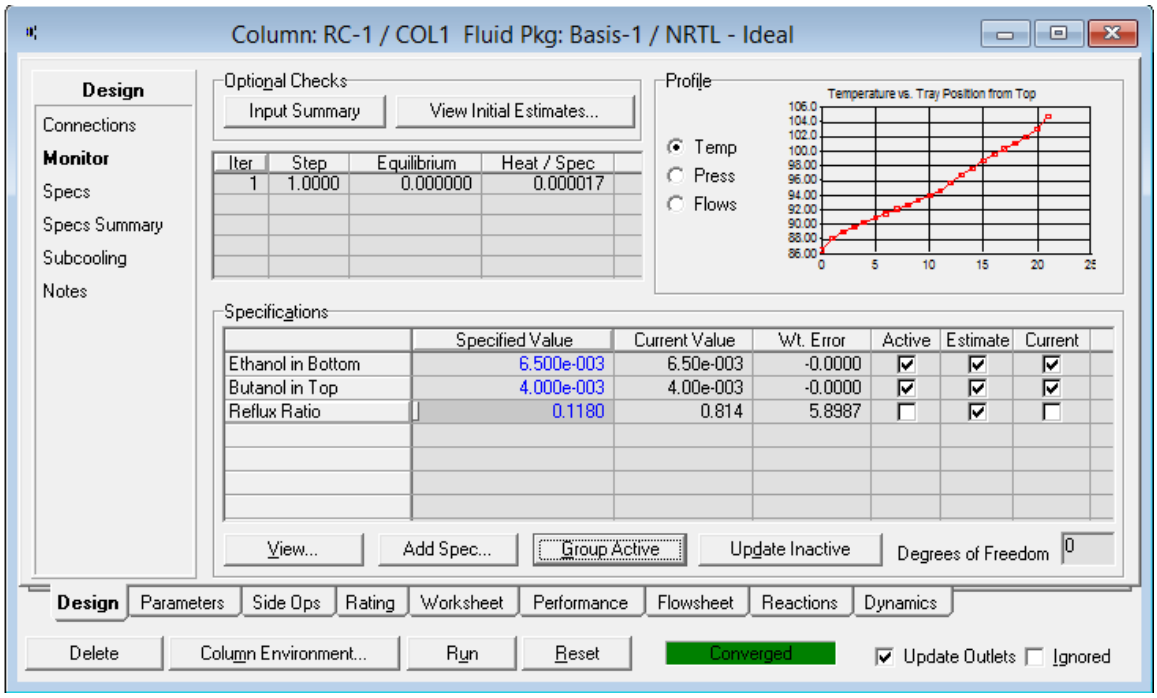


Figure 4-8: Specifications for Convergence of Column RC-1

Provide the values of light and heavy key component fraction in bottom and distillate product. After specifying these values, click on “Run” button for the convergence of column RC-1. Similarly column RC-1, add new distillation columns RC-2, RC-3 and its material streams. Define these columns by specifying number of stages, feed plate location and connecting necessary streams. Shortcut calculations of sloppy configuration will provide the initial estimate for number of stages of both these columns RC-2 and RC-3. This initial estimate for number of stages is required to carry out further simulation. The values of light component in bottom and heavy component in top streams are identified for each column. Now click the “Run” button to converge these column. The specifications for the convergence of these columns are given in the figures below.

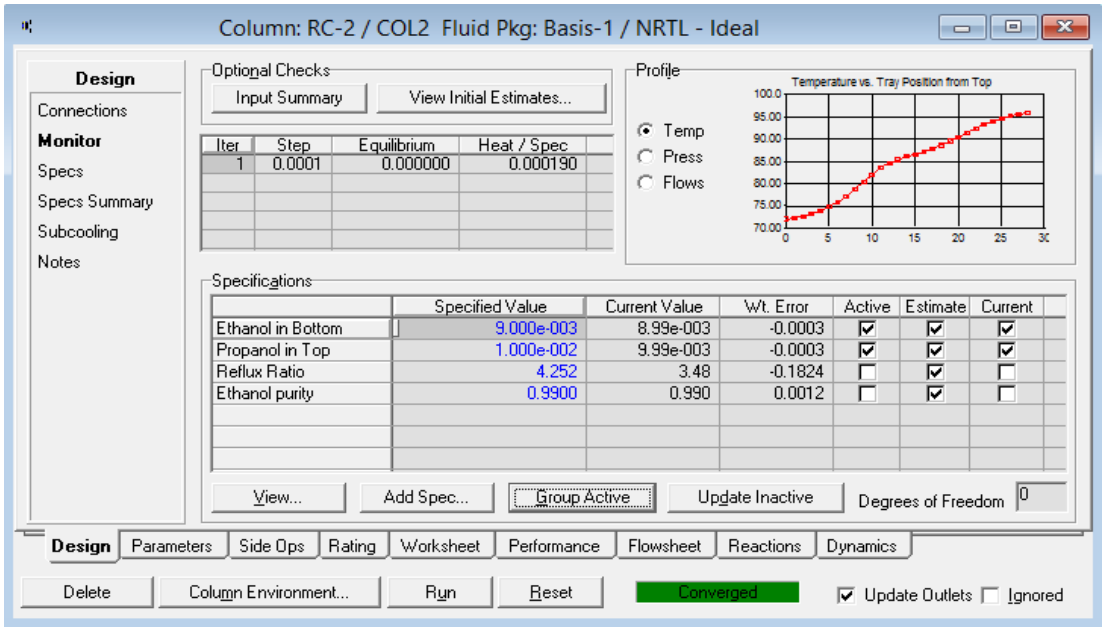


Figure 4-9: Specification for Convergence of Column RC-2

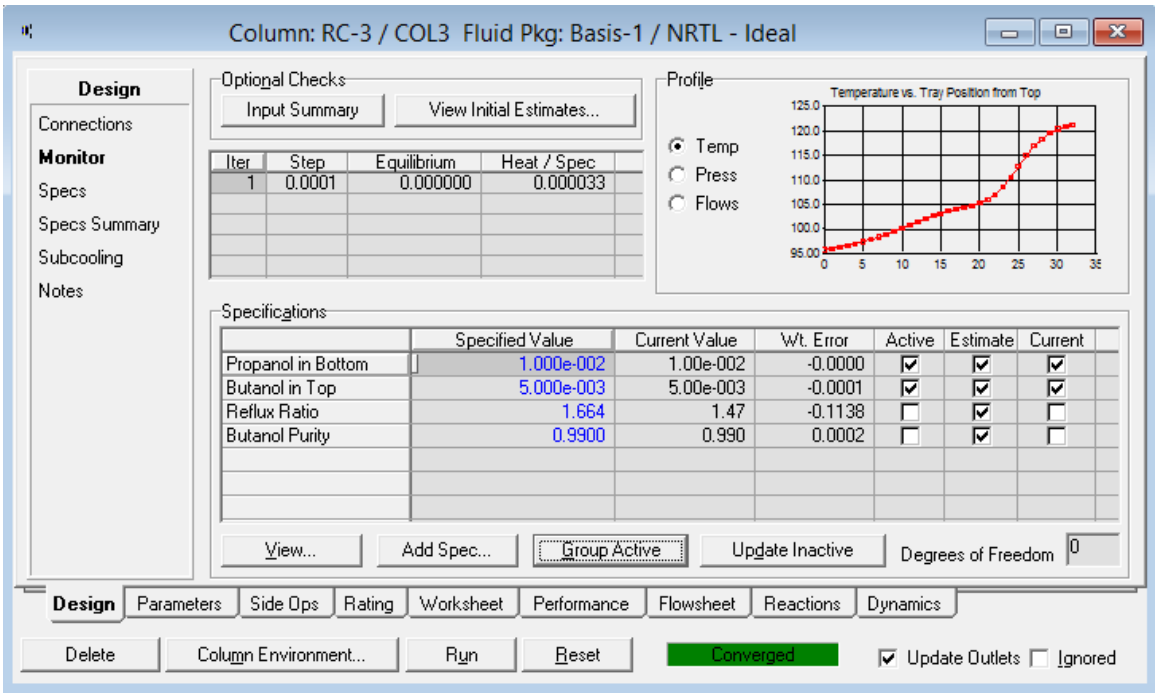


Figure 4-10: Specification for Convergence of Column RC-3

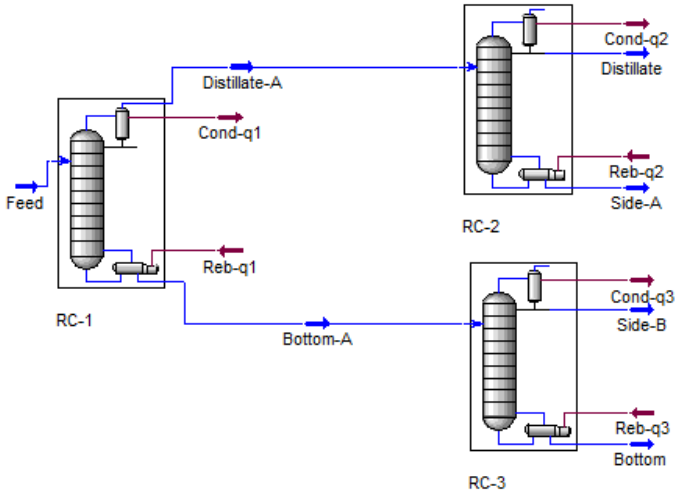
RC-1		
Number of Trays	20.00	
Duties Summary (Condenser)	-404.1	kW
Reboiler Duty	905.1	kW

Distillate-A		
Temperature	86.53	C
Pressure	88.50	kPa
Molar Flow	42.79	kgmole/h
Master Comp Mole Frac (Ethanol)	0.4587	
Master Comp Mole Frac (1-Propanol)	0.5373	
Master Comp Mole Frac (1-Butanol)	0.0040	

Feed		
Temperature	93.95	C
Pressure	100.0	kPa
Molar Flow	100.0	kgmole/h
Master Comp Mole Frac (Ethanol)	0.2000	
Master Comp Mole Frac (1-Propanol)	0.6000	
Master Comp Mole Frac (1-Butanol)	0.2000	

Bottom-A		
Temperature	104.8	C
Pressure	110.0	kPa
Molar Flow	57.21	kgmole/h
Master Comp Mole Frac (Ethanol)	0.0065	
Master Comp Mole Frac (1-Propanol)	0.6469	
Master Comp Mole Frac (1-Butanol)	0.3466	

RC-2		
Number of Trays	27.00	
Duties Summary (Condenser)	-953.4	kW
Reboiler Duty	470.8	kW



RC-3		
Number of Trays	31.00	
Duties Summary (Condenser)	-1077	kW
Reboiler Duty	1079	kW

Distillate		
Temperature	72.14	C
Molar Flow	19.62	kgmole/h
Master Comp Mole Frac (Ethanol)	0.9900	
Master Comp Mole Frac (1-Propanol)	0.0100	
Master Comp Mole Frac (1-Butanol)	0.0000	

Side-A		
Temperature	95.85	C
Molar Flow	23.17	kgmole/h
Master Comp Mole Frac (Ethanol)	0.0090	
Master Comp Mole Frac (1-Propanol)	0.9836	
Master Comp Mole Frac (1-Butanol)	0.0074	

Side-B		
Temperature	95.79	C
Molar Flow	37.37	kgmole/h
Master Comp Mole Frac (Ethanol)	0.0100	
Master Comp Mole Frac (1-Propanol)	0.9851	
Master Comp Mole Frac (1-Butanol)	0.0050	

Bottom		
Temperature	121.2	C
Molar Flow	19.84	kgmole/h
Master Comp Mole Frac (Ethanol)	0.0000	
Master Comp Mole Frac (1-Propanol)	0.0100	
Master Comp Mole Frac (1-Butanol)	0.9900	

Figure 4-11: Process Flow Sheet of Rigorous Sloppy Configuration: Alcohol Application

In this 1st step of simulation, the initial design parameters given by shortcut method are validated and the validated results are briefed in Table 4-3.

Table 4-3: Validation of Initial Design Parameters of Shortcut Method by Rigorous Simulation

Design Specifications	Shortcut Simulation	Rigorous Simulation
	Ethanol/Propanol/Butanol	Ethanol/Propanol/Butanol
Distillate		
Flow Rate (kmol/hr)	19.61	19.62
X_D (Mole fraction)	0.995/0.010/0	0.990/0.010/0
Side		
Flow Rate (kmol/hr)	60.55	60.54
X_S (Mole fraction)	0.0097/0.9844/0.0059	0.0095/0.9843/0.0062
Bottom		
Flow Rate (kmol/hr)	19.84	19.84
X_B (Mole fraction)	0/0.010/0.9900	0/0.010/0.9900
Heat Duty		
$Q_{Reboiler}$ (kW)	2203	2455
$Q_{Condenser}$ (kW)	2178	2436

It is observed that the rigorous simulation of first step proceeds to almost the similar purities which is fixed as constraints in the shortcut method. There is no any difference in the required product purity supposed in shortcut design method and resulted by the rigorous simulation. It is also observed in above table that the lighter product (top) has no any traces of heavy component and the heavier product has also no any traces of light component. Table 4-4 presented the compositions of the interlinking streams among the pre-fractionator and the main column.

Table 4-4: Compositions of Vapor and Liquid Interlinking Streams between Pre-fractionator and Main Column

	Shortcut Simulation	Rigorous Simulation
Streams	Ethanol/Propanol/Butanol	Ethanol/Propanol/Butanol
Vapour (Mole fraction)	0.4093/0.5867/0.0040	0.4587/0.5373/0.0040
Liquid (Mole fraction)	0.0064/0.6123/0.3812	0.0065/0.6469/0.3466

It is noted that the component compositions of interlinking streams between the two columns found from rigorous simulation are the same as found by shortcut method and this similarity validate the accuracy and efficiency of the proposed design method. After simulations of shortcut sloppy configuration and rigorous sloppy configuration, 2nd step of DWC simulation is carried out. The shortcut design method is based on the assumptions of constant relative volatility of any two components, negligible internal heat exchange, constant vapor and liquid molar flow rates on all stages except for the boil-up stream and reflux stream. Out of these mentioned assumptions, one or more assumption is often not valid and therefore rigorous simulation is necessary.

The initial estimates obtained from shortcut method are used to initiate the simulations to obtain the accurate design parameters. Most process simulators are designed based on equilibrium stage models because equilibrium stage models are more acceptable for ideal distillation systems [95]. The liquid and vapor streams entering and leaving each stage of column are assumed to be in equilibrium in equilibrium stage model. To start the simulation of DWC, repeat the same starting procedure as discussed in the previous section and add the components of ternary feed mixture. For VLE calculations choose NRTL thermodynamic model. After defining the components of feed mixture and thermodynamic model, enter the simulation environment and add the distillation column S-101 to the flow sheet. Then connect all the material streams for pre-fractionator (S-100) and for main column (S-101).

Two recycle blocks RCY-1 and RCY-2 are added to flow sheet for recycle streams. Inlet and outlet of RCY-1 are defined by connecting the Liquid-out A and Liquid-out B at inlet and outlet respectively. In the same way, Inlet and outlet of RCY-2 are defined by

connecting the Vapor-out A and Vapor-out B at inlet and outlet respectively. For the Pre-fractionator of DWC, select the absorber from the object palette and insert this absorber column to the HYSYS flow sheet as a pre-fractionator (S-100).

The column parameters are adjusted by connecting streams, specifying number of stages and feed plate location of Main-Vapor, Main-Liquid, Liquid-out A, Vapor-out A and Side as shown in Figure 4-12. The shortcut distillation provide an initial guess of stages for column SC-101 A and SC-101 B, in further. simulation these number of stages are equivalent to the total stages of main column of DWC. The stages number for main column of DWC are taken as 60, where 27 are the stages for SC-101A column and 31 are the stages for SC-101B column which are taken from shortcut sloppy configuration (Figure 4-6). In this simulation 2 additional stages are added due to condenser and reboiler of the DWC main column. Whenever there is a vapor liquid equilibrium in distillation column then at the same time there is a vapor and liquid equilibrium in the reboiler and condenser. Hence, in vapor liquid equilibrium phase the condenser and reboiler are considered as a tray. The feed stage of inlet streams Distillate-A and Bottom-A in shortcut columns configuration (Figure 4-6) is considered as the feed stage of Main-Vapor and Main-Liquid streams in DWC rigorous simulation.

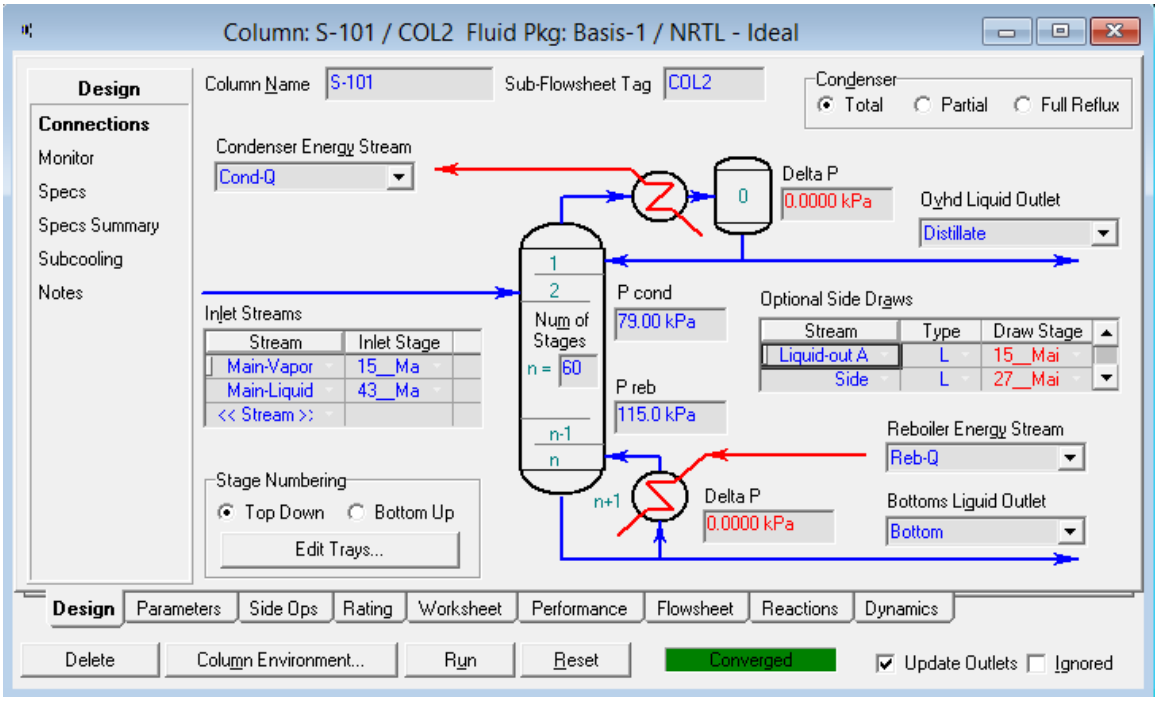


Figure 4-12: Input Parameters for DWC Main column

1st shortcut column SC-101A (Figure 4-6) has 27 number of stages and the side product is drawn from the last stage of column SC-101A, therefore stage number 27 is taken as the side stream draw location. The energy streams Reb-Q and Cond-Q are added to DWC main column S-101 and then the flow sheet will be completed as shown in Figure 4-12. There are five degrees of freedom for main column (S-101) of the DWC. A classic distillation column having reboiler, condenser, bottom and distillate streams has two degree of freedom [95]. For every side stream, the degree of freedom of column will increase by one. As main column of DWC has three side streams (Liquid-out A, Side, Vapor-out A), so its degree of freedom is five and these degrees of freedom are used to specify the flow rates and required purity of all products. These five specifications includes the product purity in each stream, boil-up and reflux rate in main column. The product purity in each stream, namely as ethanol purity, propanol purity and butanol purity in Distillate, Side and Bottom streams respectively are specified as three active specifications of the column.

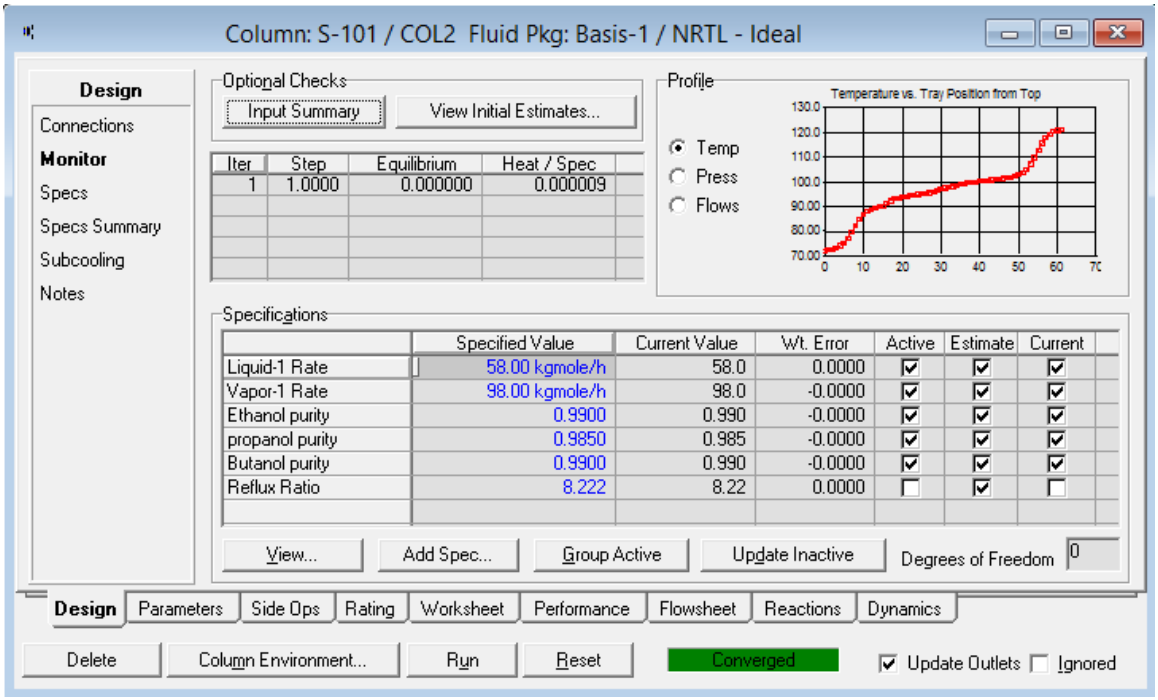


Figure 4-13: Specifications for Convergence of DWC Main Column

The flow rate of vapor and liquid streams are also added as remaining two specifications and then column specifications are completed. Now activate column simulation calculations and click on the "Run", the column converges after many iterations.

The simulation data for pre-fractionator is provided for its convergence by simulation. The input data needed to converge pre-fractionator (S-100) is shown in Figure 4-14. The complete DWC flow sheet will converge after a long iterations.

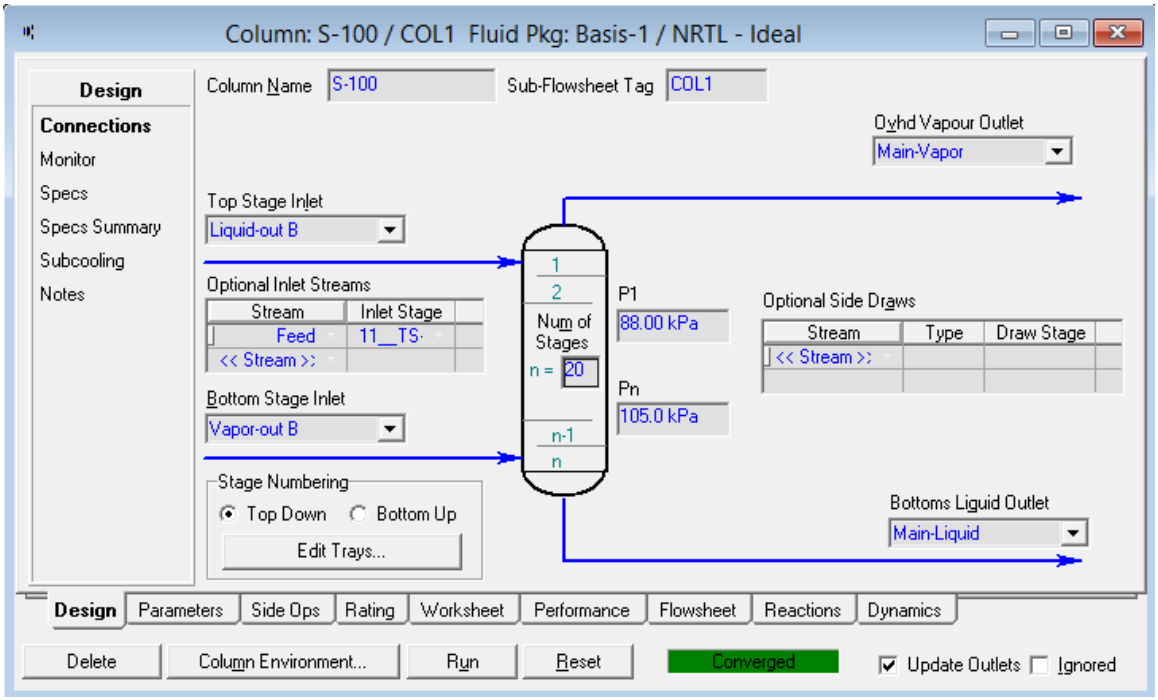
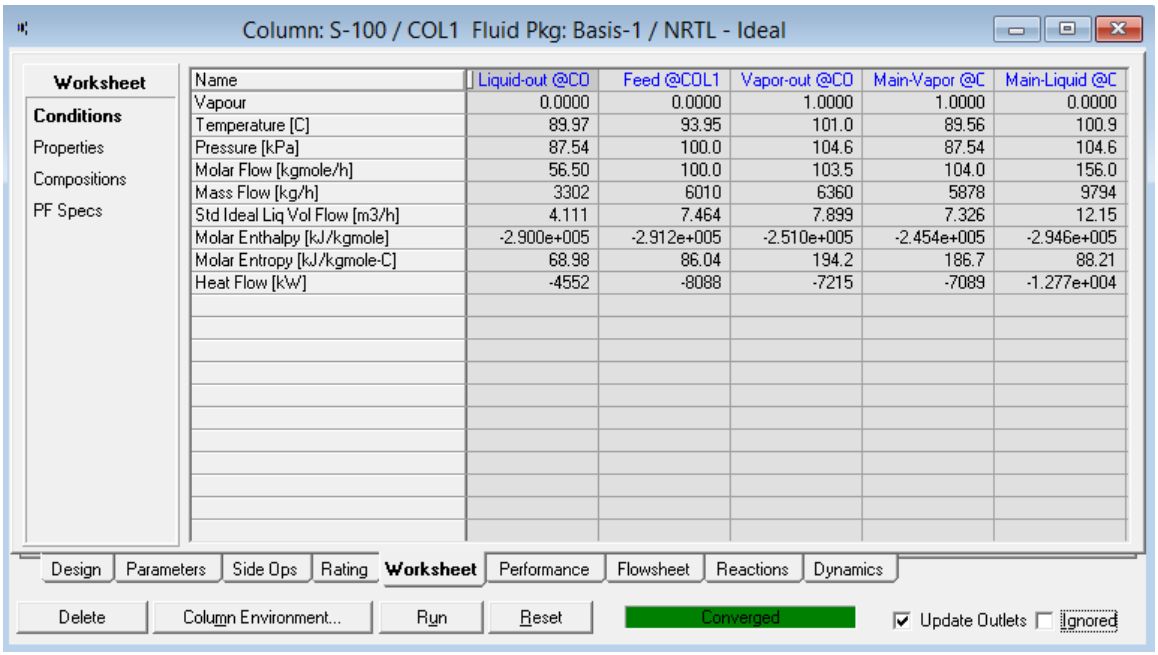


Figure 4-14: Input Data for Convergence of Pre-Fractionator



Name	Liquid-out @C0	Feed @COL1	Vapor-out @C0	Main-Vapor @C	Main-Liquid @C
Vapour	0.0000	0.0000	1.0000	1.0000	0.0000
Temperature [C]	89.97	93.95	101.0	89.56	100.9
Pressure [kPa]	87.54	100.0	104.6	87.54	104.6
Molar Flow [kgmole/h]	56.50	100.0	103.5	104.0	156.0
Mass Flow [kg/h]	3302	6010	6360	5878	9794
Std Ideal Liq Vol Flow [m3/h]	4.111	7.464	7.899	7.326	12.15
Molar Enthalpy [kJ/kgmole]	-2.900e+005	-2.912e+005	-2.510e+005	-2.454e+005	-2.946e+005
Molar Entropy [kJ/kgmole-C]	68.98	86.04	194.2	186.7	88.21
Heat Flow [kW]	-4552	-8088	-7215	-7089	-1.277e+004

Figure 4-15: Complete Worksheet of Pre-fractionator

Complete worksheet of Pre-fractionator (S-100) is shown in Figure 4-15 and flow sheet of converged DWC along with technical data and simulation results is given in Figure 4-16. There are total four case studies considered for design and simulation studies of DWC and

these case studies are taken form the literature. The feed specifications, product specifications and other operating conditions for these case studies are provided in Table 4-5.

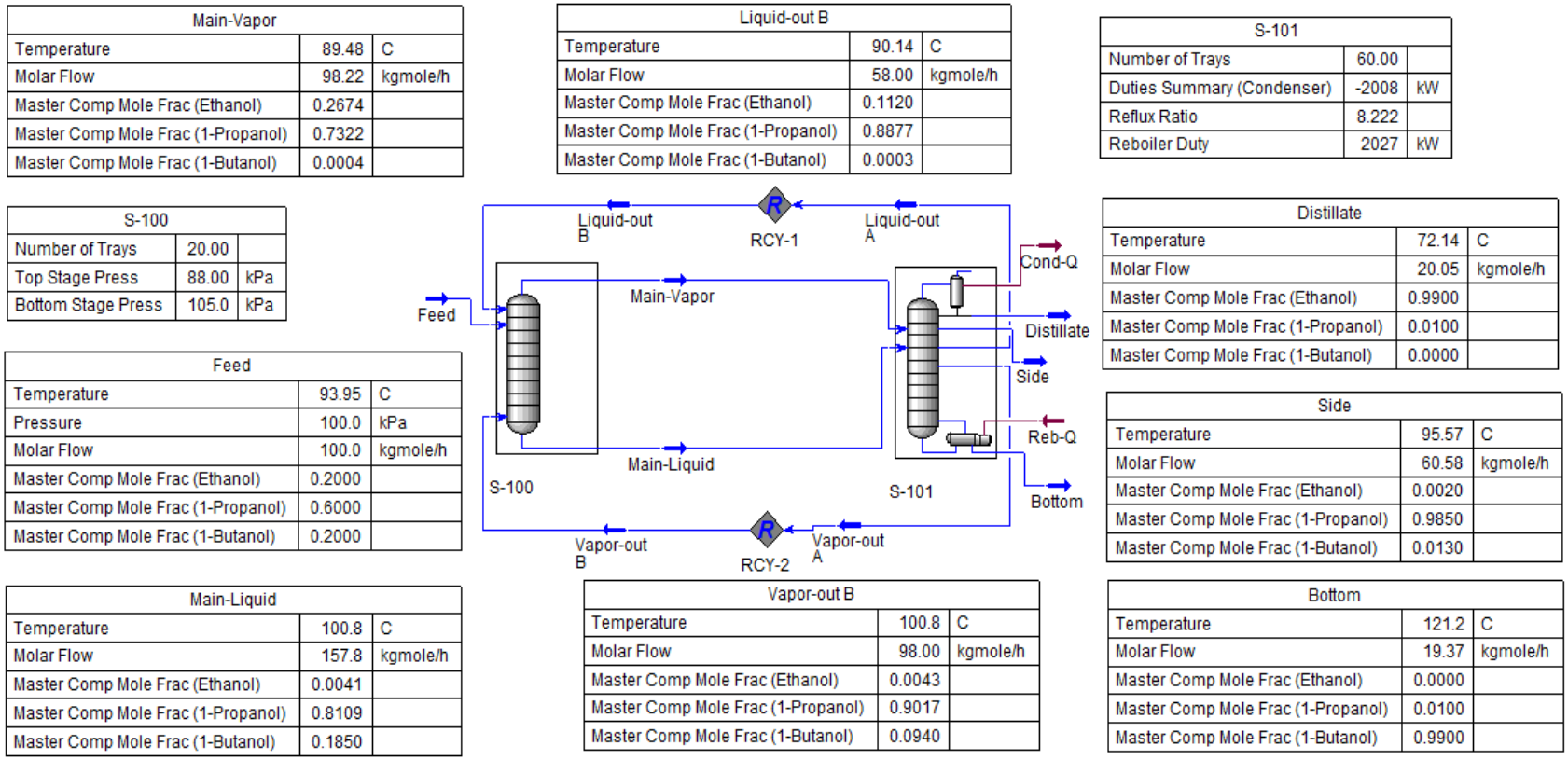


Figure 4-16: Flow Sheet of Converged DWC: Alcohol Application (Non-optimal results)

4.5 Optimization of DWC

The structure of DWC design that is obtained as a result of rigorous simulation is not the finally optimized design structure. There is a need to optimize the DWC design in order to find the minimum reboiler duty for energy efficient operation of DWC. During distillation operation, any reduction in reboiler duty could result in minimum operating cost. Hence, design structure of DWC is optimized by optimizing the internal flow distribution of liquid and vapor in the main column of DWC.

In this optimization study, the objective function is to minimize the reboiler duty of the column and the optimization constraint is the product purity of the components. During optimization process, the product purity should not be disturbed. Optimization of the DWC by using HYSYS DataBook is described below for alcohol application. HYSYS DataBook could be used to evaluate key variables under different process scenarios, and finds the results in graphical or tabular format. To start the optimization procedure, open the DataBook from the Tools menu in HYSYS flow sheet. The first step in optimization is to add the process key variables to DataBook through Variables tab. For this alcohol application, the internal flow distribution of liquid and vapor are varied to examine its effect on the following key variables:

- Reboiler heat duty
- Condenser heat duty

In DataBook view, click the Insert tab and then Variable Navigator view will appears. Select S-101 (main column) in the Object list, and the list of Variables available for the main column S-101 will appear at the right hand side of the Object list. Now select Spec Value option in the Variables list and specification list will appear in the Variable Specifics table. Select Liquid-1 Rate from the

Variable Specifics list and click OK. The selected variable now appear in the DataBook view. In order to add the new variable, again click the Insert tab and repeat the same procedure as discussed above to select the Vapor-1 Rate from the Variables Specifics list and press OK as shown in the figure below.

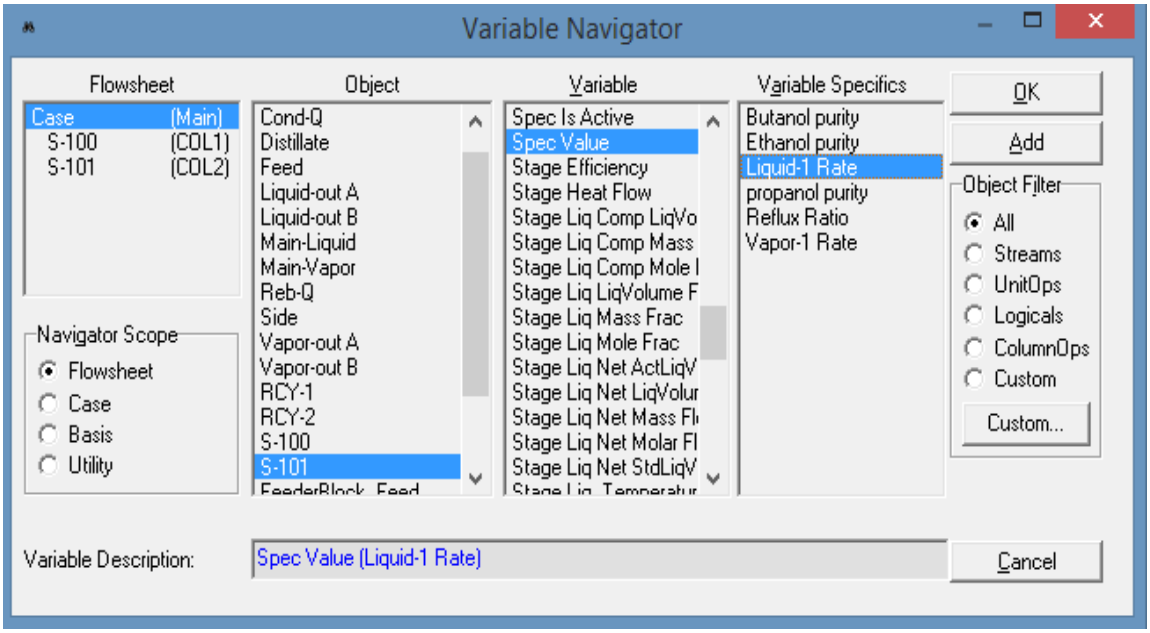


Figure 4-17: DataBook Variable Navigator View in Hysys

The new variable will appears in the DataBook view. Click the insert tab again to add the third variable condenser duty. Select Cond-Q from the Object list and Heat flow from the Variable list and then press OK to add this variable in the DataBook. Similarly to add the last fourth variable, repeat the same procedure to select Reb-Q from the Object list and add this variable to DataBook view. The Variables tab of the DataBook with four variables are given below.

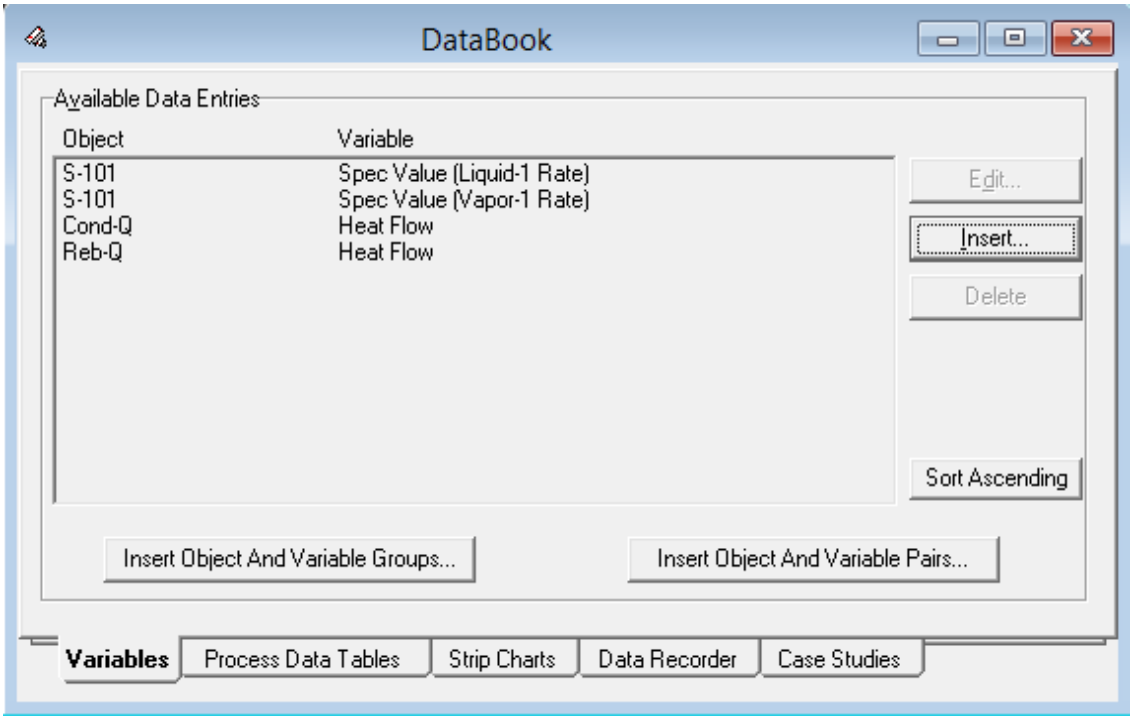


Figure 4-18: DataBook with Process Variables for Optimization

After adding these process variables to the DataBook, the next phase is to generate a data table to show these key variables. To generate the data table, select the Process Data Tables tab and then select the Add button. HYSYS will generate a new data table with built in name ProcData1 and Activate all the variables by selecting the corresponding small boxes. Now click on Case Studies tab and select Add button in Available Case Studies group. HYSYS will generate a new table with default name Case Study 1. Then change the default name to DWC Energy Optimization. Now activate the variables as independent and dependent variable by clicking on the corresponding checkbox. The internal flow distribution of liquid and vapor (Liquid-1 & Vapor-1) are selected as independent variables and heat duties of condenser and reboiler (Cond-Q & Reb-Q) are selected as dependent variables. By variation in internal flow distribution of liquid and vapor, the reboiler heat duty will also changes. The completed DataBook view is given below in Figure 4-19.

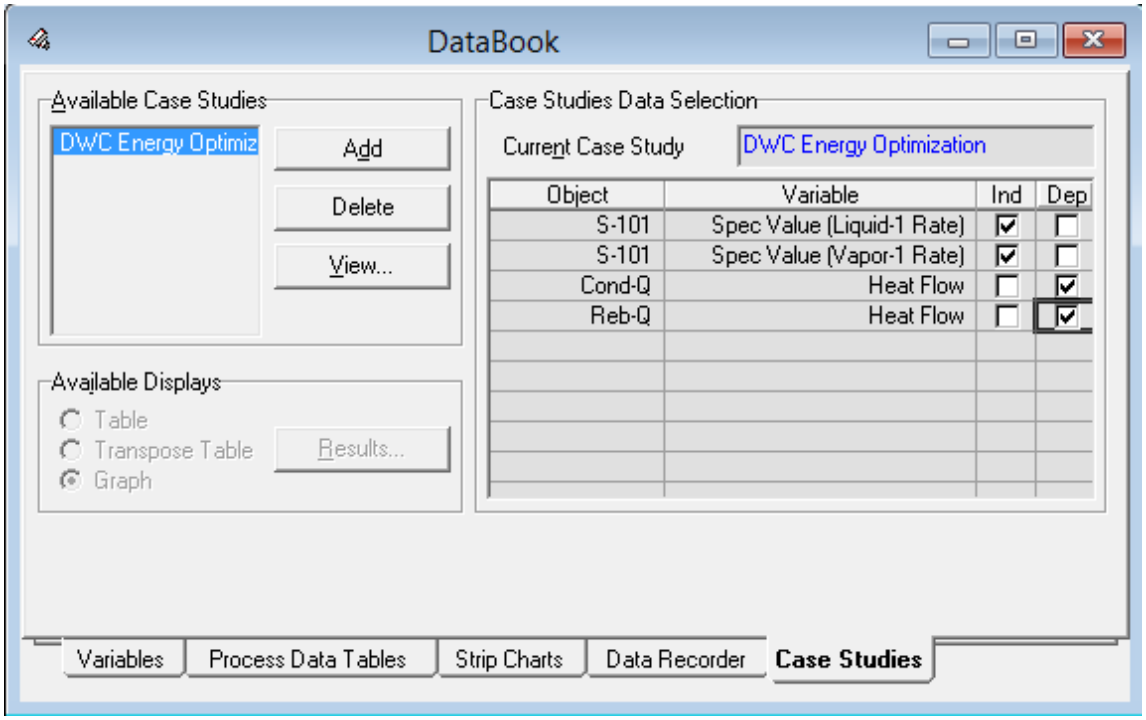


Figure 4-19: Independent and Dependent Key Variables in DWC Energy Optimization

Now click on View tab in Available Case Studies, a new table will open. In this table, suitable values of Low Bound, High Bound and Step Size of the independent variables to be enter. Now click on Start button to start the optimization process. The long simulation calculations will start and click on Results tab in Available Displays to observe the optimization results in graphical form. Figure 4-20 shows the input data given for low and high bound ranges of liquid and vapor flow distribution for this alcohol separation case study. This optimization takes several minutes to execute (3721 number of states) and by the changing in internal flow distribution the significant changes in graph could be observed during optimization.

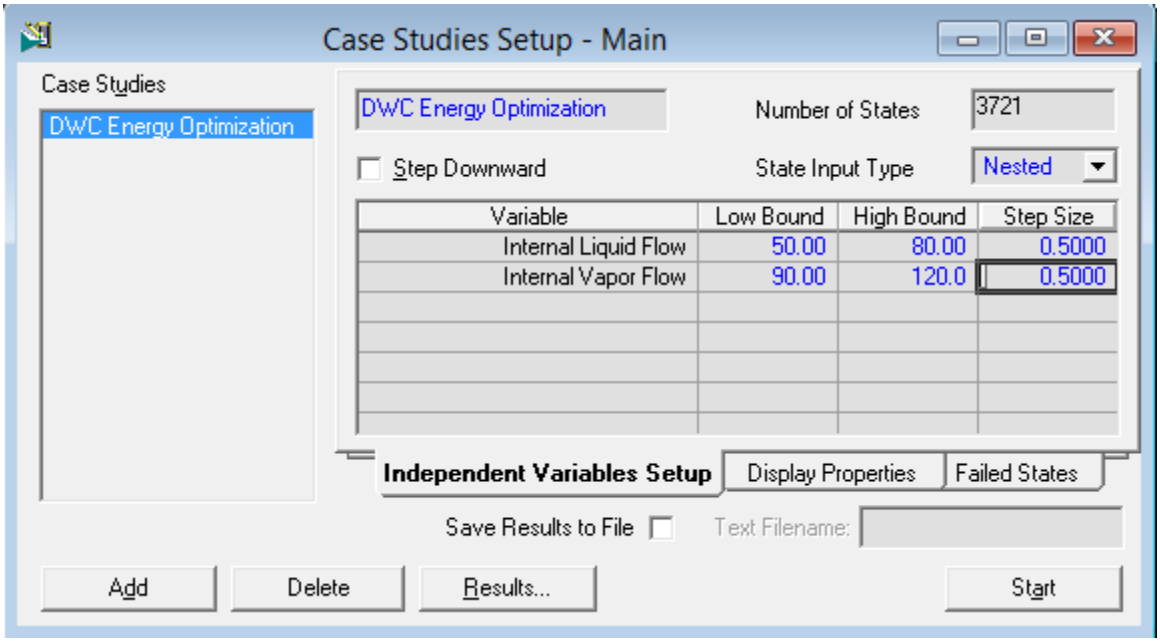


Figure 4-20: Range of Liquid and Vapor Flow Distribution for Optimization

After completion of 3721 optimization states, click on Table option to investigate the optimum values of the liquid and vapor flow distribution corresponding to the minimum reboiler heat duty. The value of the minimum energy consumption results the optimum values of the internal flow distribution of liquid and vapor.

The impact of internal flow distribution on DWC reboiler duty is represented in Figure 4-21. The figure shows that there is a presence of an optimized internal flow distribution that gives the minimum reboiler duty. The figure also illustrates that the reboiler heat duty is very sensitive to liquid and vapor flow distribution. Normally, the internal flow distribution of liquid and vapor in DWC are the extreme critical design parameters that affects the separation efficiency and energy requirement among all other key variables.

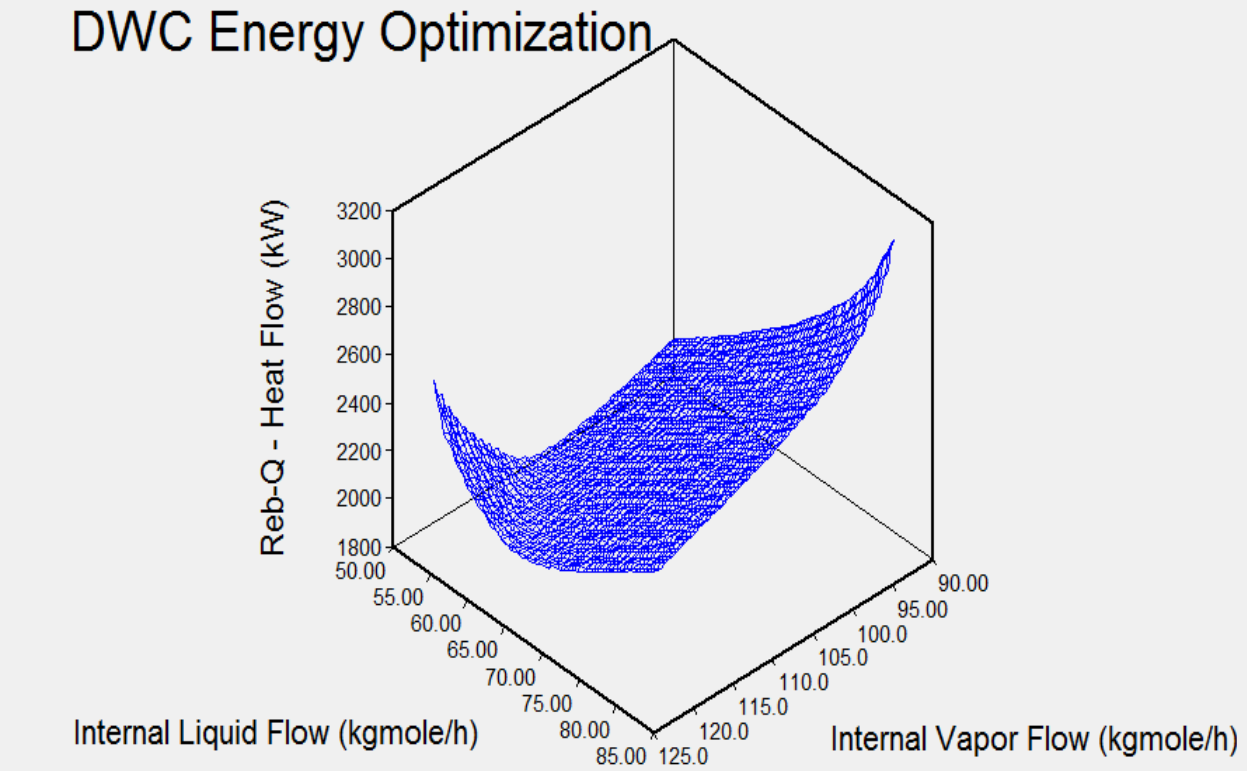


Figure 4-21: Variation in Energy Consumption with Variable Internal Flow Distribution

For this alcohol application, the minimum energy consumption after optimization is 1927 kW when internal liquid and vapor flow distribution are 56.5 kmol/h and 103.5 kmol/h respectively. Therefore, any variation in internal flow distribution from optimal flow conditions could results in a sensitive and asymmetrical effect on separation efficiency and energy efficiency. Figure 4-22 represents the technical data and simulation results of DWC after optimization for BTE application.

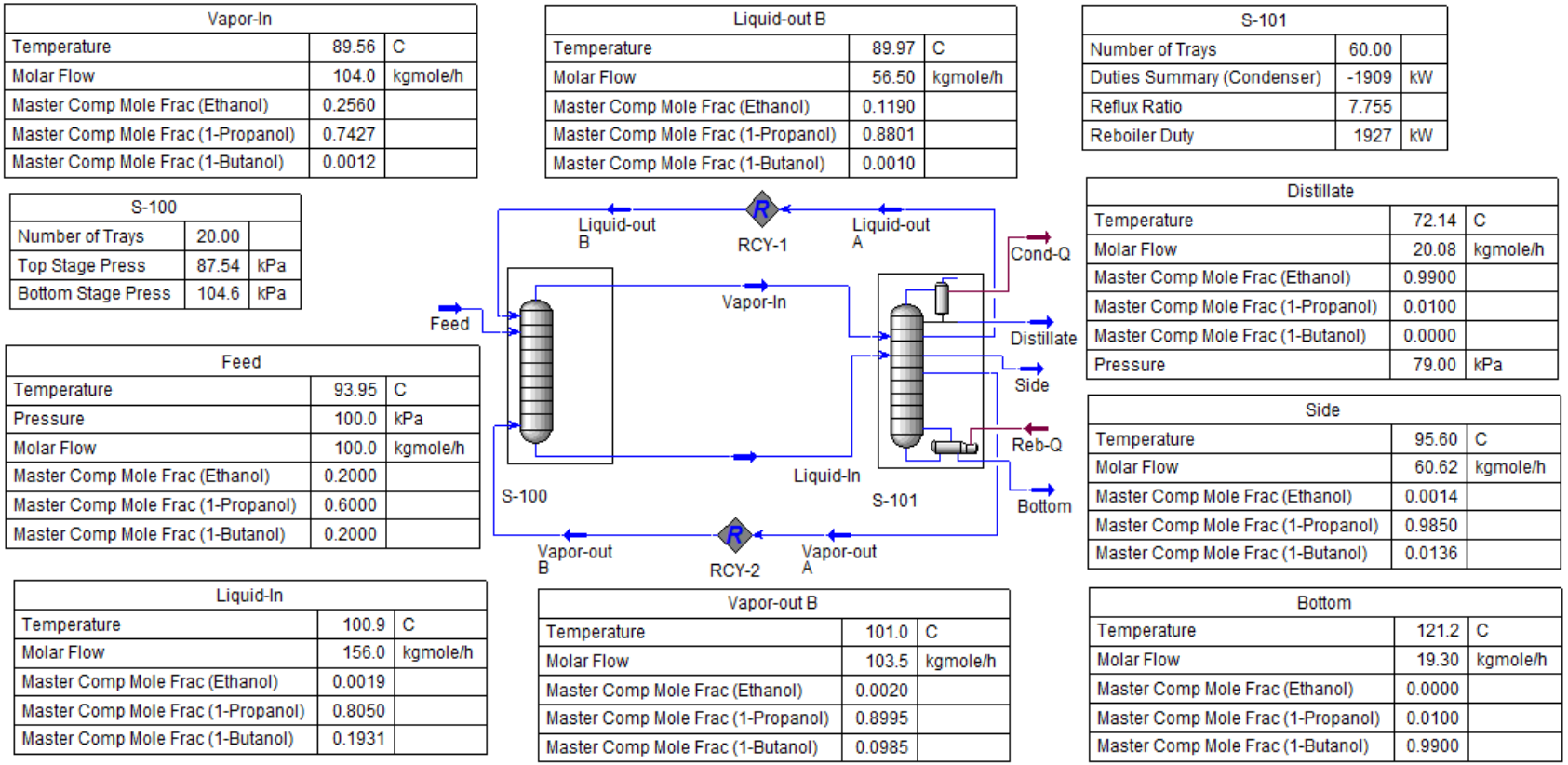


Figure 4-22: Flow Sheet of Optimized DWC: Alcohol application

4.6 Graphical Results of Optimized DWC

After optimization of DWC structure, the results were analyzed. These results are presented in the graphical form. Figure 4-23 and 4-24 represents the comparison of the temperature and composition profiles for 1st rigorous column in rigorous sloppy configuration and the pre-fractionator of DWC.

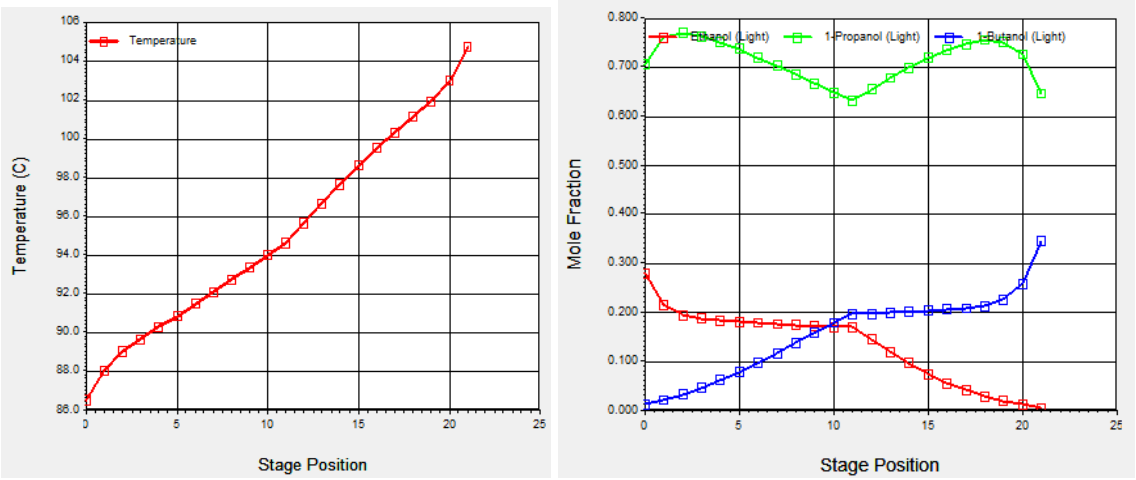


Figure 4-23: Temperature and Composition Profile vs. Tray position for 1st Rigorous Column

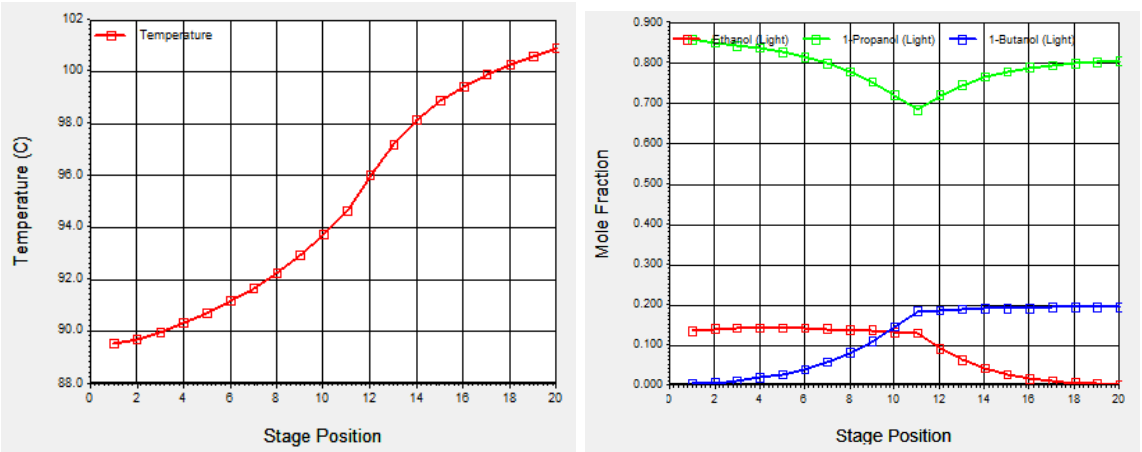


Figure 4-24: Temperature and Composition Profile vs. Tray Position for DWC Pre-fractionator

The comparison shows the similarity in composition profile and temperature profile. In Figure 4-24, the composition of ethanol and propanol increasing from tray 11 (feed tray) to top of the pre-fractionator whereas the concentration of propanol and butanol increasing

from feed tray towards the bottom of pre-fractionator. The equal distribution of middle component propanol to both ends of pre-fractionator leads to significant energy reduction for multicomponent separation process.

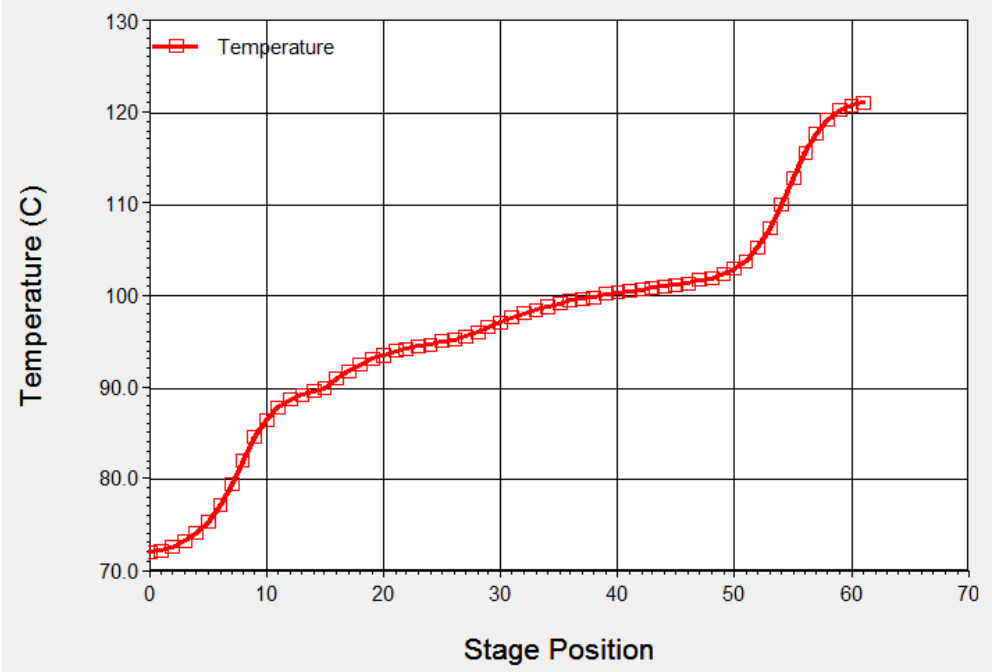


Figure 4-25: Temperature Profile vs. Tray Position for DWC Main Column

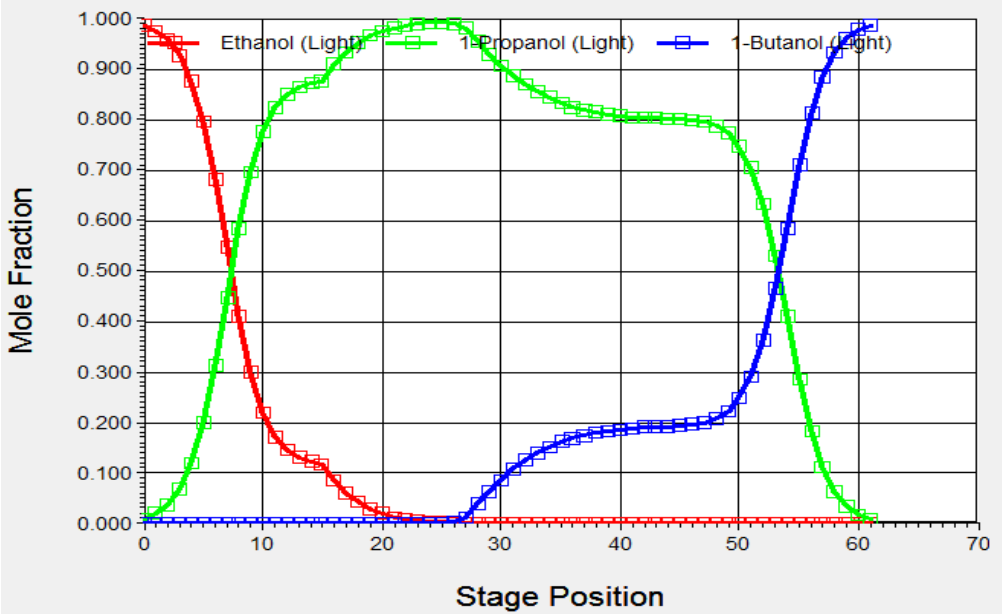


Figure 4-26: Composition Profile vs. Tray Position for DWC Main Column

The temperature profile of the DWC main column is presented in Figure 4-25, the temperature is increasing continuously from top stage (condenser) towards bottom stage (reboiler).

The composition profile of ternary mixture for the main column of DWC is shown in Figure 4-26. According to the figure, the molar concentration of ethanol increases continuously from tray 15 towards the top of column and its concentration is maximum (99%) at the top plate, while the concentration of butanol is increasing towards the bottom of the column and highest (99%) at the lower plate. The molar concentration of propanol is increasing from top towards middle and from bottom to middle of the column, the maximum concentration of propanol (98.5%) is at tray 27 which is the draw tray location of the side stream.

Although the composition and temperature profiles of the 2^{nd} and 3^{rd} rigorous shortcut column are not shown here, the similarity in the profiles between the sloppy configuration and DWC has been seen. This also indicates the validity of the structure similarity among DWC and sloppy configurations.

In Figure 4-27, the internal flow rates of liquid and vapor in main column of DWC are presented. The vapor flow rate shows a sudden increase of 104 kmol/h on tray 15 corresponding to the vapor feed stage and decrease to 0 kmol/h in the condenser at the column top. Similarly, the liquid flow rate shows a sharp increase of 156 kmol/h on tray 43 corresponding to the liquid feed stage and a sharp decrease at the bottom of column in the reboiler.

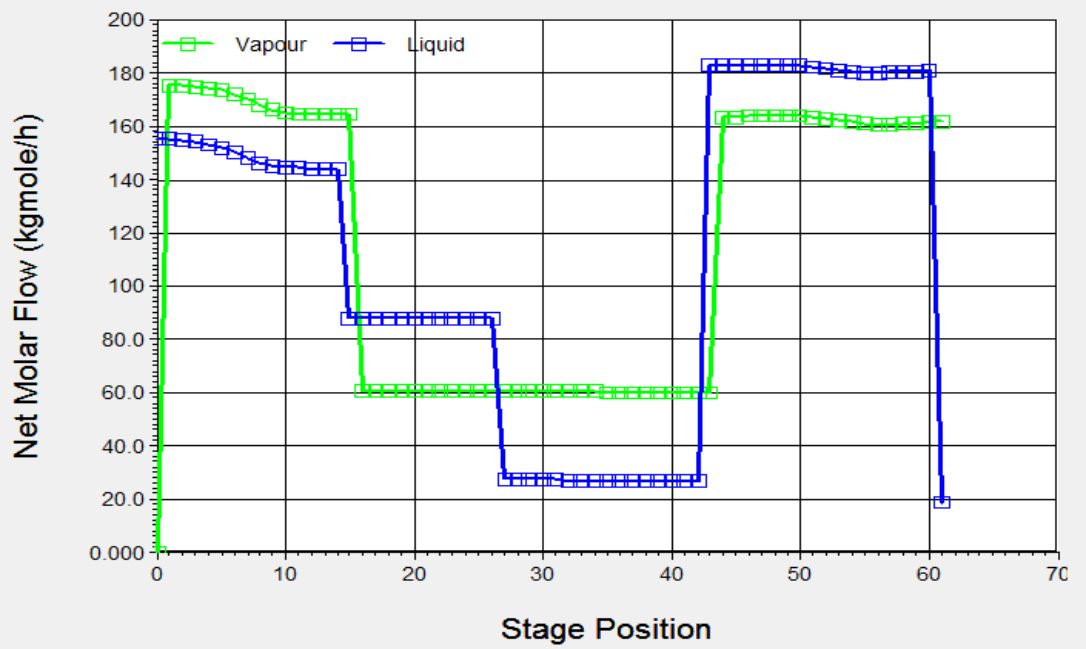


Figure 4-27: Molar Vapor and Liquid Flows in DWC Main Column

4.7 Effect of Energy Supply on Product Compositions in DWC

This section presents the study of the effect of available energy supply (reboiler heat duty) on composition of column products, when the distillation column is operated at energy lower than the optimum energy required for the optimized operation of the DWC. For this analysis, the optimal design of DWC for alcohol application is considered. Then DWC is operated at different values of energy that are lower than the optimal value of energy required for the optimal operation. The effect of lowering the reboiler energy has been investigated on composition of side product in main column of DWC. The ternary mixture composition profile for optimal operation of DWC (alcohol application) is shown in Figure 4-26.

4.7.1 DWC Operation at Different Values of Lower Energy than Optimal Energy

To investigate the influence of available energy supply on the side product composition, the DWC is operated at available energy of 5%, 10%, 15% and 20% lower than original optimal value. The composition profiles of DWC main column for all these cases are given below.

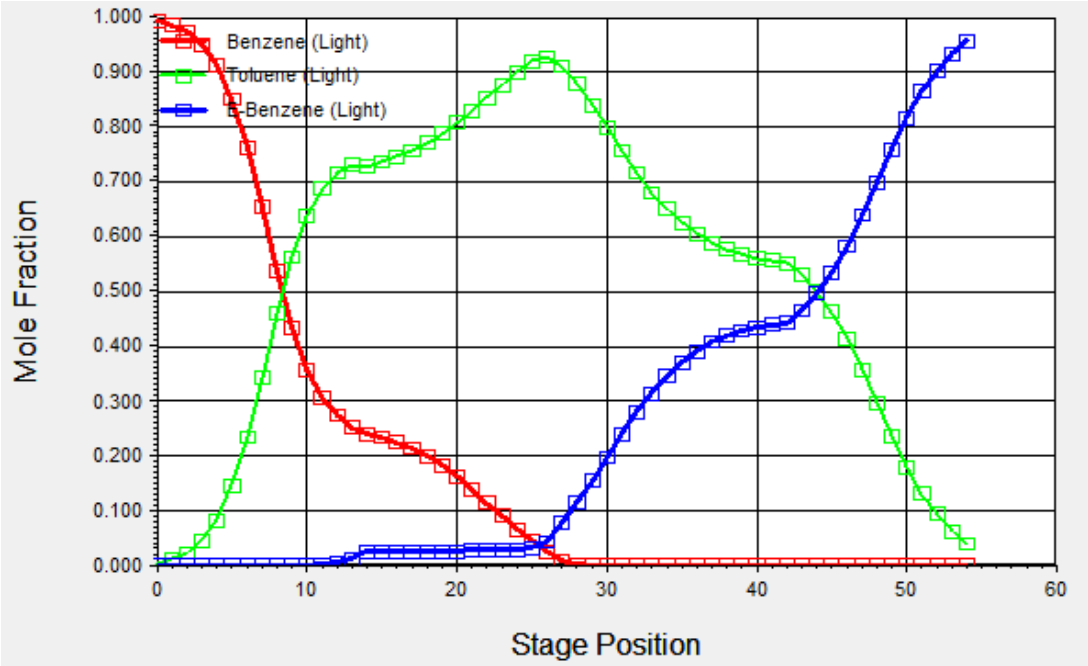


Figure 4-28: Composition Profile for DWC Main Column (5% lower energy)

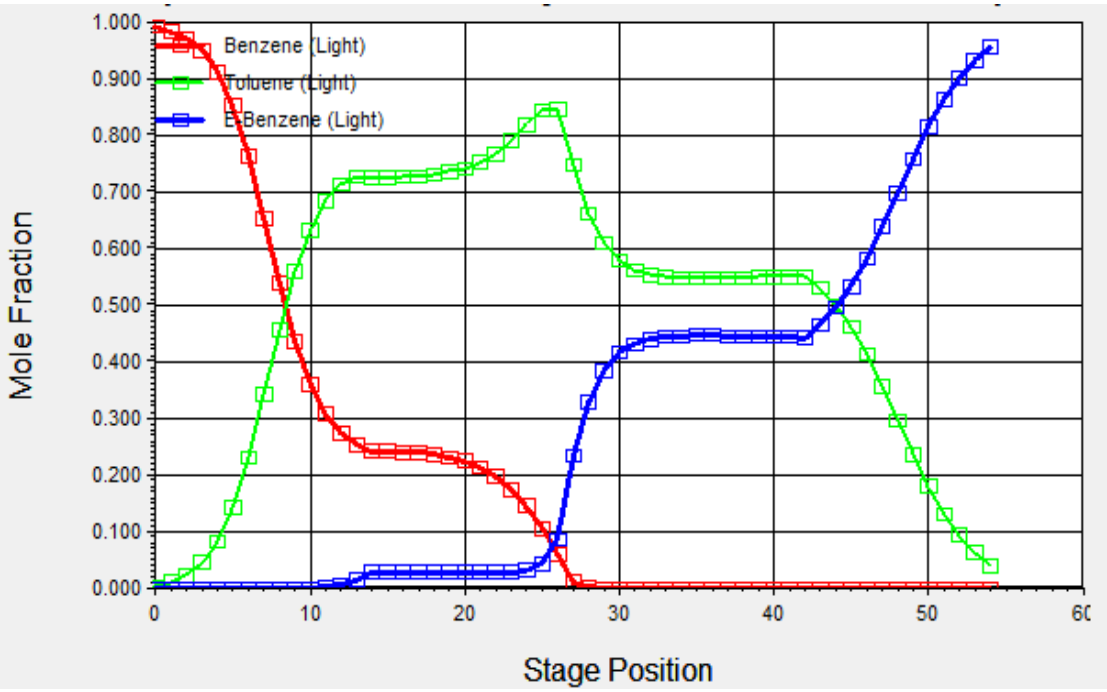


Figure 4-29: Composition Profile for DWC Main Column (10% lower energy)

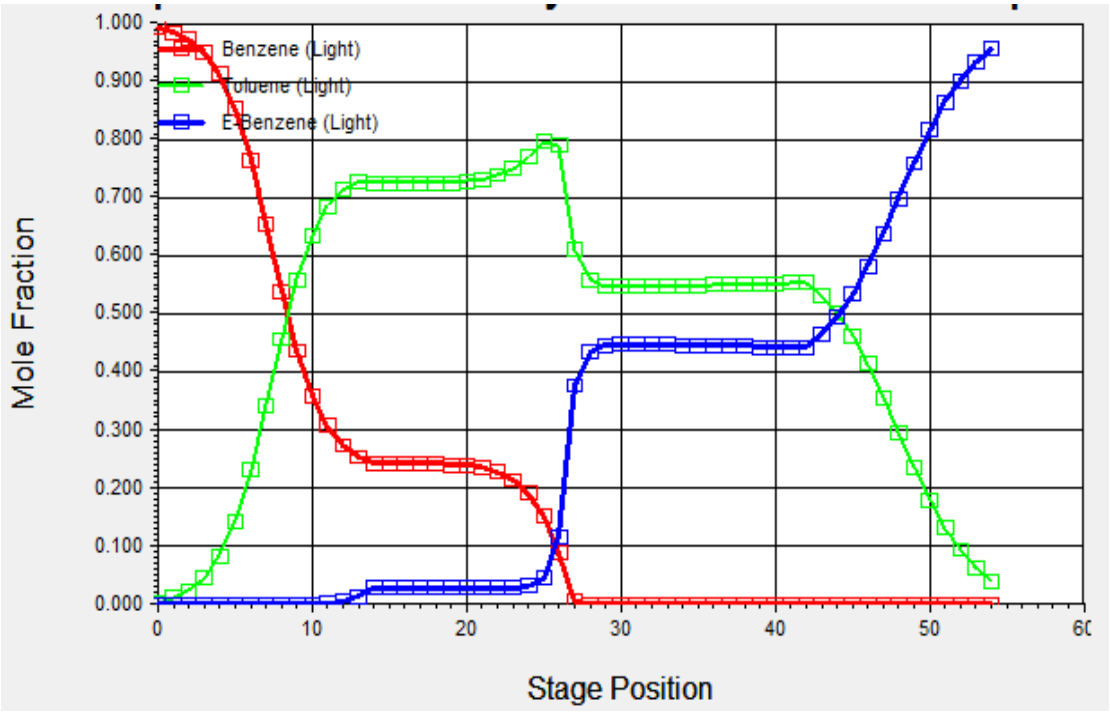


Figure 4-30: Composition Profile for DWC Main Column (15% lower energy)

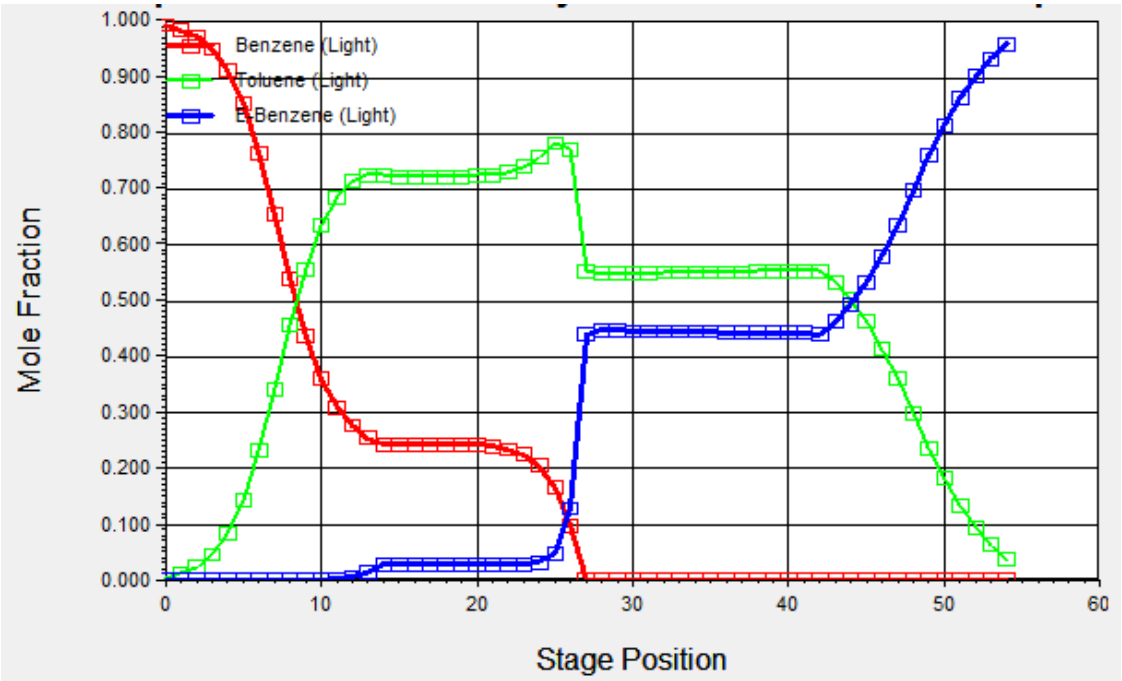


Figure 4-31: Composition Profile for DWC Main Column (20% lower energy)

4.7.2 Results

The analysis has been carried out to observe the purity of the DWC side product for different values of the reboiler duty. Figure 4-28 to 4-31 clearly represents that the energy consumption can directly disturb the side product purity while the top product purity and bottom product purity remains the same. There is a very negligible change in the purity of top and bottom product but by supplying less energy than the optimal energy required to run the column, the purity of side product will decrease. When we decrease the energy than the optimal energy value, we can no longer stick to the required composition of the side product.

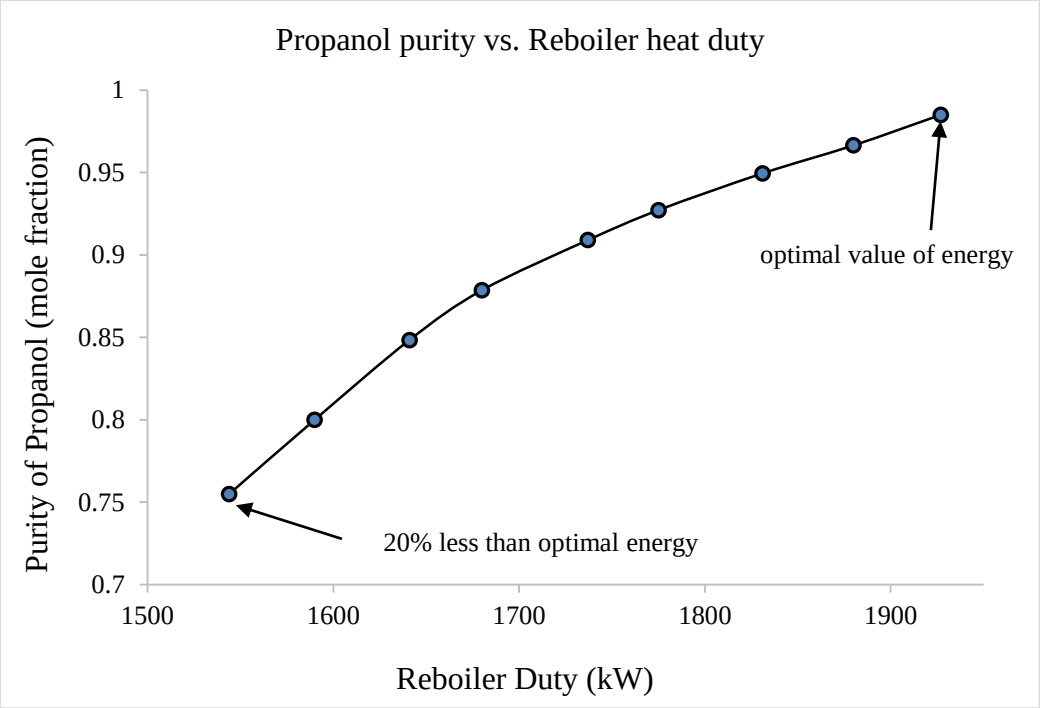


Figure 4-32: Propanol Purity vs. Reboiler Duty of DWC: Alcohol Application

Figure 4-32 shows the graphical representation of reduction in purity of side product by variation in the range of the reboiler duty lower than the energy needed for optimal operation of the DWC.

Table 4-5: Characteristics of Different DWC Application Studied for Simulation

Characteristics of the DWC Application Studied for Simulation						
#	**Components**	**Feed Composition**	**Feed Conditions**	**Product Specifications (Mole %)**	**Other Conditions**	**Literature Reference**
1	**Alcohol Separation**					
	Ethanol	0.20	100 kgmol/h	Ethanol: 99%	Column Pressure: 1 bar	Hassiba et al (2015)
	Propanol	0.60	1 bar saturated liquid (q=1)	Propanol: 98.5%	Total Condenser	
	Butanol	0.20		Butanol: 99%	NRTL Model	
2	**BTX Separation**					
	Benzene	0.30	3600 kgmol/h	Benzene: 99%	Column Pressure: 37 kPa	Hassiba et al (2015)
	Toluene	0.30	37 kPa saturated liquid (q=1)	Toluene: 98.5%	Total Condenser	
	p-Xylene	0.40		p-Xylene: 99%	Peng-Robinson Model	
3	**BTE Separation**					
	Benzene	0.33	100 kgmol/h	Benzene: 99.5%	Column Pressure: 1.75 bar	Bek-Pedersen et al. (2004)
	Toluene	0.33	1.75 bar saturated liquid (q=1)	Toluene: 96%	Total Condenser	
	Ethyl Benzene	0.34		Ethyl Benzene: 96%	Peng-Robinson Model	
4	**Alkane Separation**					
	n-Pentane	0.4	45 kgmol/h	n-Pentane: 99.5%	Column Pressure: 1.49 bar	Benyounes et al. (2015)
	n-Hexane	0.2	1.49 bar saturated liquid (q=1)	n-Hexane: 98.5%	Total Condenser	
	n-Heptane	0.4		n-Heptane: 92%	Peng-Robinson Model	

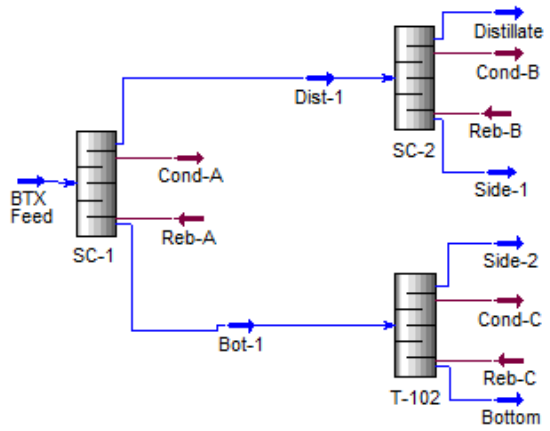
Dist-1		
Temperature	54.61	C
Pressure	28.00	kPa
Molar Flow	1541	kgmole/h
Master Comp Mole Frac (Benzene)	0.6967	
Master Comp Mole Frac (Toluene)	0.3003	
Master Comp Mole Frac (p-Xylene)	0.0030	

Bot-1		
Temperature	96.36	C
Pressure	40.00	kPa
Molar Flow	2059	kgmole/h
Master Comp Mole Frac (Benzene)	0.0030	
Master Comp Mole Frac (Toluene)	0.2998	
Master Comp Mole Frac (p-Xylene)	0.6972	

Distillate		
Temperature	27.91	C
Pressure	15.00	kPa
Molar Flow	1082	kgmole/h
Master Comp Mole Frac (Benzene)	0.9900	
Master Comp Mole Frac (Toluene)	0.0100	
Master Comp Mole Frac (p-Xylene)	0.0000	

Side-1		
Temperature	66.94	C
Molar Flow	458.9	kgmole/h
Master Comp Mole Frac (Benzene)	0.0050	
Master Comp Mole Frac (Toluene)	0.9849	
Master Comp Mole Frac (p-Xylene)	0.0101	

BTX Feed		
Temperature	71.72	C
Pressure	37.00	kPa
Molar Flow	3600	kgmole/h
Master Comp Mole Frac (Benzene)	0.3000	
Master Comp Mole Frac (Toluene)	0.3000	
Master Comp Mole Frac (p-Xylene)	0.4000	



Side-2		
Temperature	66.63	C
Molar Flow	611.9	kgmole/h
Master Comp Mole Frac (Benzene)	0.0101	
Master Comp Mole Frac (Toluene)	0.9849	
Master Comp Mole Frac (p-Xylene)	0.0050	

SC-1		
Minimum Reflux	0.5126	
Minimum Trays	5.686	
Actual Trays	15.39	
Optimal Feed	8.151	
Condenser Duty	-9157	kW
Reboiler Duty	2.479e+004	kW

SC-2		
Minimum Reflux	1.169	
Minimum Trays	9.446	
Actual Trays	22.56	
Optimal Feed	7.810	
Condenser Duty	-2.365e+004	kW
Reboiler Duty	8815	kW

T-102		
Minimum Reflux	2.208	
Minimum Trays	10.91	
Actual Trays	24.48	
Optimal Feed	16.01	
Condenser Duty	-2.188e+004	kW
Reboiler Duty	2.156e+004	kW

Bottom		
Temperature	102.9	C
Pressure	35.00	kPa
Molar Flow	1447	kgmole/h
Master Comp Mole Frac (Benzene)	0.0000	
Master Comp Mole Frac (Toluene)	0.0100	
Master Comp Mole Frac (p-Xylene)	0.9900	

Figure 4-33: Flow Sheet of Converged Shortcut Sloppy Configuration: BTX Application

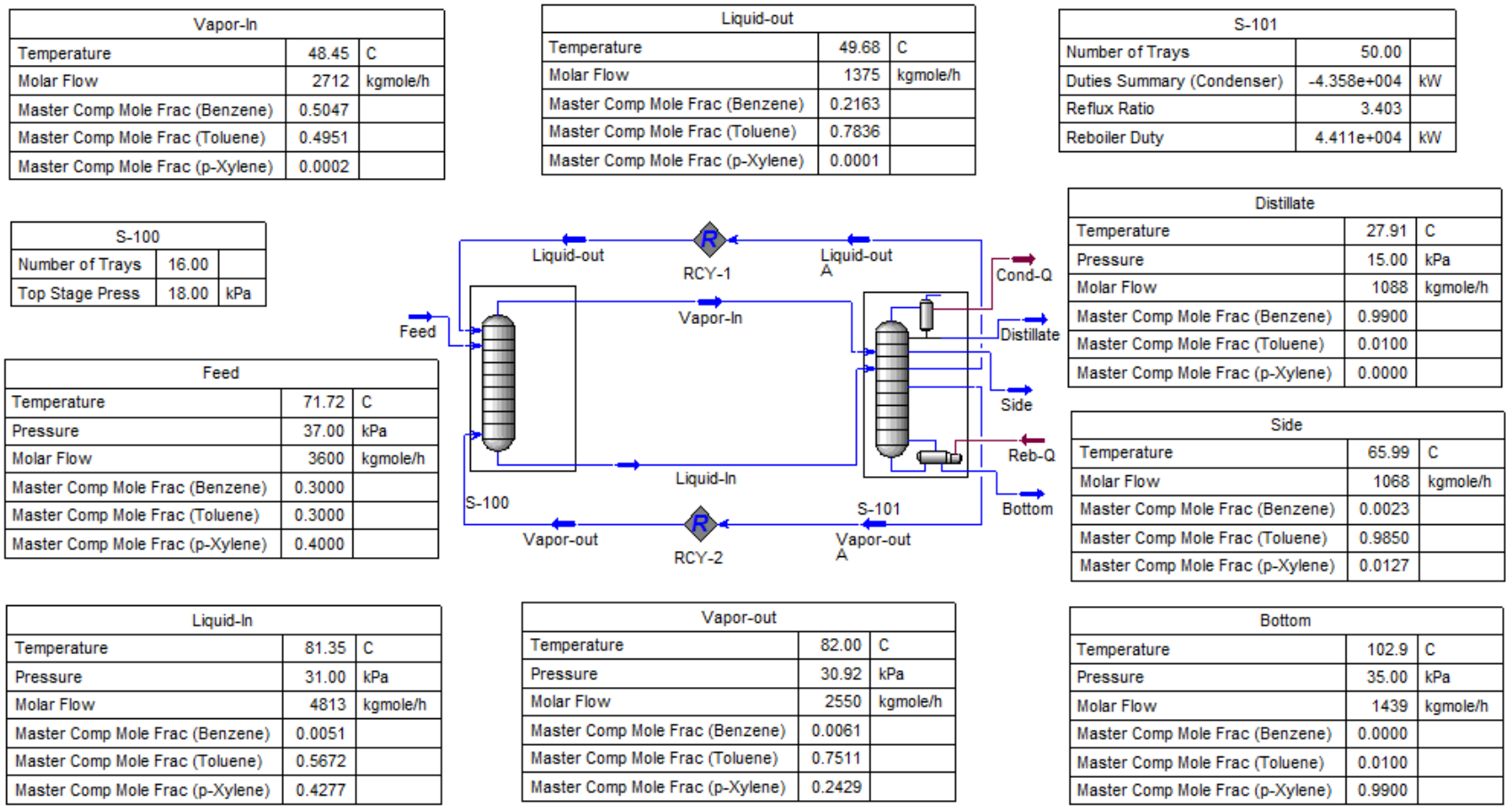


Figure 4-34: Flow Sheet of Optimized DWC: BTX Application

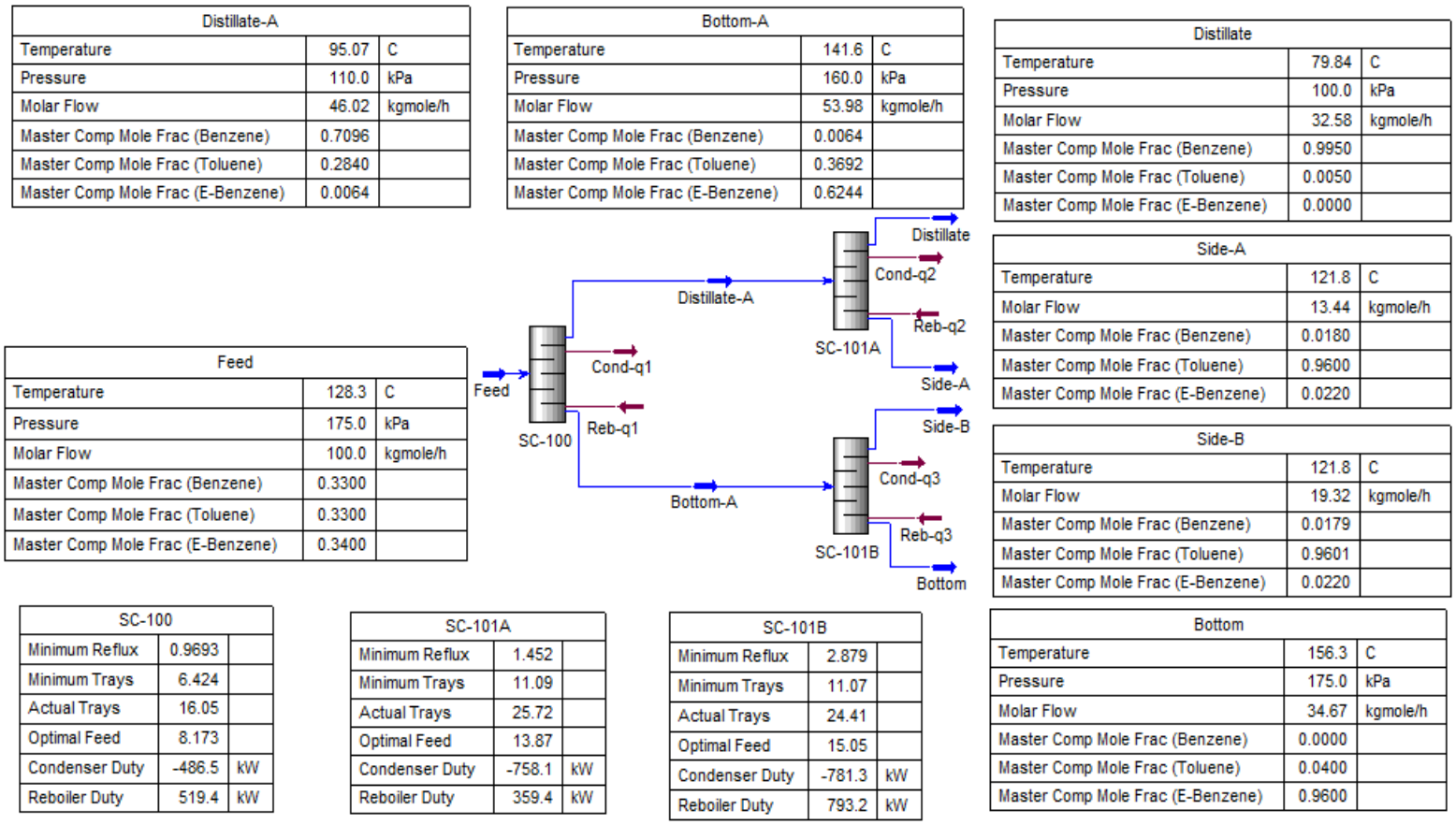


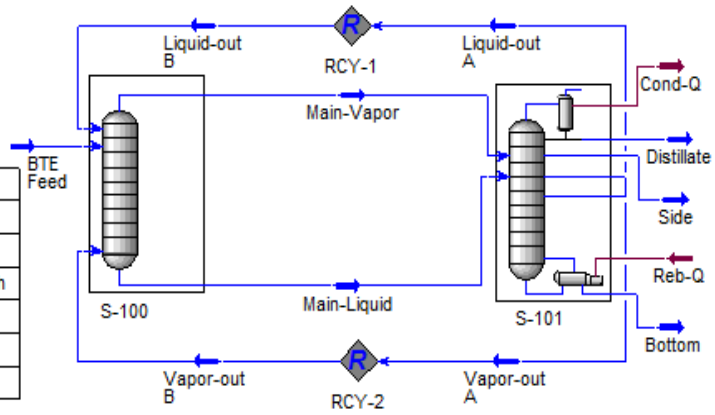
Figure 4-35: Flow Sheet of Converged Shortcut Sloppy Configuration: BTE Application

Main-Vapor		
Temperature	110.1	C
Pressure	130.0	kPa
Molar Flow	110.9	kgmole/h
Master Comp Mole Frac (Benzene)	0.4251	
Master Comp Mole Frac (Toluene)	0.5555	
Master Comp Mole Frac (E-Benzene)	0.0194	

Liquid-out B		
Temperature	112.4	C
Pressure	140.0	kPa
Molar Flow	58.00	kgmole/h
Master Comp Mole Frac (Benzene)	0.2458	
Master Comp Mole Frac (Toluene)	0.7320	
Master Comp Mole Frac (E-Benzene)	0.0222	

S-101		
Number of Trays	53.00	
Top Stage Press	120.0	kPa
Duties Summary (Condenser)	-1325	kW
Reboiler Duty	1345	kW

S-100		
Number of Trays	17.00	
Bottom Stage Press	190.0	kPa



Distillate		
Temperature	85.94	C
Pressure	120.0	kPa
Molar Flow	32.97	kgmole/h
Master Comp Mole Frac (Benzene)	0.9950	
Master Comp Mole Frac (Toluene)	0.0050	
Master Comp Mole Frac (E-Benzene)	0.0000	

BTE Feed		
Temperature	128.3	C
Pressure	200.0	kPa
Molar Flow	100.0	kgmole/h
Master Comp Mole Frac (Benzene)	0.3300	
Master Comp Mole Frac (Toluene)	0.3300	
Master Comp Mole Frac (E-Benzene)	0.3400	

Side		
Temperature	127.4	C
Pressure	158.5	kPa
Molar Flow	32.02	kgmole/h
Master Comp Mole Frac (Benzene)	0.0053	
Master Comp Mole Frac (Toluene)	0.9600	
Master Comp Mole Frac (E-Benzene)	0.0347	

Main-Liquid		
Temperature	143.6	C
Pressure	190.0	kPa
Molar Flow	154.1	kgmole/h
Master Comp Mole Frac (Benzene)	0.0027	
Master Comp Mole Frac (Toluene)	0.5753	
Master Comp Mole Frac (E-Benzene)	0.4221	

Vapor-out B		
Temperature	142.6	C
Pressure	183.1	kPa
Molar Flow	107.0	kgmole/h
Master Comp Mole Frac (Benzene)	0.0028	
Master Comp Mole Frac (Toluene)	0.6991	
Master Comp Mole Frac (E-Benzene)	0.2981	

Bottom		
Temperature	162.0	C
Pressure	200.0	kPa
Molar Flow	34.01	kgmole/h
Master Comp Mole Frac (Benzene)	0.0000	
Master Comp Mole Frac (Toluene)	0.0400	
Master Comp Mole Frac (E-Benzene)	0.9600	

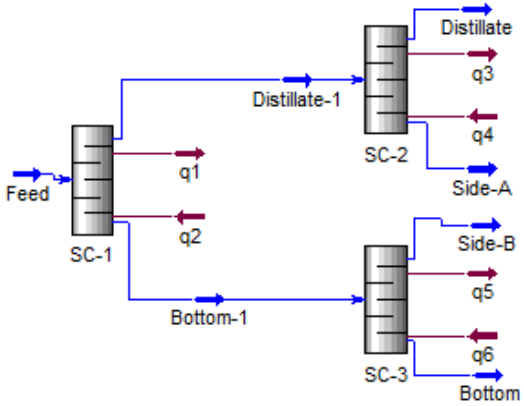
Figure 4-36: Flow Sheet of Optimized DWC: BTE Application

Distillate-1		
Temperature	48.43	C
Molar Flow	22.17	kgmole/h
Master Comp Mole Frac (n-Pentane)	0.8110	
Master Comp Mole Frac (n-Hexane)	0.1880	
Master Comp Mole Frac (n-Heptane)	0.0010	

Bottom-1		
Temperature	98.69	C
Molar Flow	22.83	kgmole/h
Master Comp Mole Frac (n-Pentane)	0.0010	
Master Comp Mole Frac (n-Hexane)	0.2117	
Master Comp Mole Frac (n-Heptane)	0.7873	

Distillate		
Temperature	37.50	C
Molar Flow	18.12	kgmole/h
Master Comp Mole Frac (n-Pentane)	0.9900	
Master Comp Mole Frac (n-Hexane)	0.0100	
Master Comp Mole Frac (n-Heptane)	0.0000	

Feed		
Temperature	70.45	C
Pressure	149.0	kPa
Molar Flow	45.00	kgmole/h
Master Comp Mole Frac (n-Pentane)	0.4000	
Master Comp Mole Frac (n-Hexane)	0.2000	
Master Comp Mole Frac (n-Heptane)	0.4000	



Side-A		
Temperature	74.17	C
Molar Flow	4.044	kgmole/h
Master Comp Mole Frac (n-Pentane)	0.0090	
Master Comp Mole Frac (n-Hexane)	0.9855	
Master Comp Mole Frac (n-Heptane)	0.0055	

Side-B		
Temperature	74.48	C
Molar Flow	4.722	kgmole/h
Master Comp Mole Frac (n-Pentane)	0.0048	
Master Comp Mole Frac (n-Hexane)	0.9852	
Master Comp Mole Frac (n-Heptane)	0.0100	

SC-1		
Minimum Reflux	0.4884	
Minimum Trays	7.328	
Actual Trays	19.56	
Optimal Feed	9.805	
Condenser Duty	-102.5	kW
Reboiler Duty	281.8	kW

SC-2		
Minimum Reflux	0.8807	
Minimum Trays	9.133	
Actual Trays	22.47	
Optimal Feed	7.690	
Condenser Duty	-268.5	kW
Reboiler Duty	103.6	kW

SC-3		
Minimum Reflux	3.726	
Minimum Trays	11.39	
Actual Trays	24.71	
Optimal Feed	15.66	
Condenser Duty	-206.5	kW
Reboiler Duty	211.7	kW

Bottom		
Temperature	108.2	C
Molar Flow	18.11	kgmole/h
Master Comp Mole Frac (n-Pentane)	0.0000	
Master Comp Mole Frac (n-Hexane)	0.0100	
Master Comp Mole Frac (n-Heptane)	0.9900	

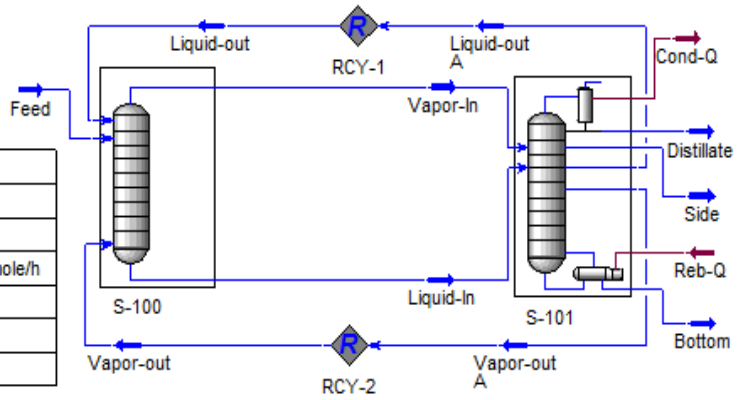
Figure 4-37: Flow Sheet of Converged Shortcut Sloppy Configuration: Alkanes Application

vAPOR-iN		
Temperature	54.23	C
Pressure	109.3	kPa
Molar Flow	37.05	kgmole/h
Master Comp Mole Frac (n-Pentane)	0.6531	
Master Comp Mole Frac (n-Hexane)	0.3468	
Master Comp Mole Frac (n-Heptane)	0.0001	

Liquid-out		
Temperature	56.27	C
Pressure	109.3	kPa
Molar Flow	18.00	kgmole/h
Master Comp Mole Frac (n-Pentane)	0.3479	
Master Comp Mole Frac (n-Hexane)	0.6521	
Master Comp Mole Frac (n-Heptane)	0.0001	

S-101		
Number of Trays	50.00	
Duties Summary (Condenser)	-452.2	kW
Reboiler Duty	471.6	kW

S-100		
Number of Trays	20.00	
Top Stage Press	109.3	kPa



Distillate		
Temperature	37.50	C
Pressure	105.0	kPa
Molar Flow	18.16	kgmole/h
Master Comp Mole Frac (n-Pentane)	0.9900	
Master Comp Mole Frac (n-Hexane)	0.0100	
Master Comp Mole Frac (n-Heptane)	0.0000	

Feed		
Temperature	70.45	C
Pressure	149.0	kPa
Molar Flow	45.00	kgmole/h
Master Comp Mole Frac (n-Pentane)	0.4000	
Master Comp Mole Frac (n-Hexane)	0.2000	
Master Comp Mole Frac (n-Heptane)	0.4000	

Side		
Temperature	74.29	C
Molar Flow	8.775	kgmole/h
Master Comp Mole Frac (n-Pentane)	0.0016	
Master Comp Mole Frac (n-Hexane)	0.9850	
Master Comp Mole Frac (n-Heptane)	0.0134	

Liquid-In		
Temperature	87.82	C
Pressure	128.3	kPa
Molar Flow	60.95	kgmole/h
Master Comp Mole Frac (n-Pentane)	0.0033	
Master Comp Mole Frac (n-Hexane)	0.5298	
Master Comp Mole Frac (n-Heptane)	0.4669	

Vapor-out		
Temperature	88.71	C
Pressure	128.3	kPa
Molar Flow	35.00	kgmole/h
Master Comp Mole Frac (n-Pentane)	0.0040	
Master Comp Mole Frac (n-Hexane)	0.6973	
Master Comp Mole Frac (n-Heptane)	0.2987	

Bottom		
Temperature	108.2	C
Pressure	135.0	kPa
Molar Flow	18.06	kgmole/h
Master Comp Mole Frac (n-Pentane)	0.0000	
Master Comp Mole Frac (n-Hexane)	0.0100	
Master Comp Mole Frac (n-Heptane)	0.9900	

Figure 4-38: Flow Sheet of Optimized DWC: Alkanes Application

4.8 Validation of DWC Simulation Design Results with Literature

After performing the simulation studies to obtain the DWC design structure for all the four case studies, it is very necessary to compare the design results obtained from simulation with the literature from where we have taken all these case studies. The simulation results and the literature results are compared in Table 4-6 below.

The comparison of the simulation results with the literature results shows that the design results which are obtained by using the proposed design method are very close or similar to those results which are given in the literature. The literature results were obtained by designing the DWC using different differential equations methods which are very lengthy and time consuming methods. The validation of the simulation design results with the literature results illustrates that the proposed design method works well and feasible to find the optimal design parameters of the DWC.

4.9 Effect of Variable Feed Composition on DWC Thermal Efficiency

This section presents the analysis of DWC thermal efficiency with variable feed composition of benzene, toluene and ethyl-benzene (BTE) mixture. The extensive simulation studies were performed to analyze the effect of feed composition on thermal efficiency of DWC by varying the molar concentration of middle boiling component (toluene) in feed. For variable molar concentration of toluene, its composition is varied in the range of 20% to 80% in ternary feed. For this investigation, the same design procedure is used to simulate the DWC as discussed above. The analyzed results are illustrated in Table 4-7. The obtained results exhibits that by using DWC for separating mixture of variable feed composition, the percentage of energy saving is increasing with the increase of toluene concentration in the feed.

Table 4-6: Comparison of Simulation Results with Literature Results

	Alcohol Application		BTX Application		Alkanes Application		BTE Application	
Parameters	**Simulation Results**	**Literature Results**	**Simulation Results**	**Literature Results**	**Simulation Results**	**Literature Results**	**Simulation Results**	**Literature Results**
Reboiler Duty (kW)	1983	2027	44,110	44,056	473	471	1345	1335
Cond. Duty (kW)	1963	1990	43,580	47,805	453	436	1325	1310
D	20	20.05	1088	1091	18.16	18	32.97	33.0
S	60	60.58	1068	1066	8.71	9	32.02	32.85
B	20	19.37	1439	1444	18.03	18	34.01	34.15
S_L	0.2075	0.35	0.3711	0.391	0.451	0.493	0.460	.490
S_V	0.442	0.574	0.6	0.55	0.6942	0.7771	0.746	.765
RR	8.13	7.75	3.4	2.84	2.461	2.59	3.780	3.94
N_{Total}	62	60	50	45	50	50	53	58
N_{Rect}	18	15	8	10	8	5	14	16
N_{Strip}	16	17	10	12	11	9	11	12
N_{pf}	28	28	27	23	31	35	28	30
N_{feed}	14	11	9	10	10	15	9	11
N_{Side}	25	27	22	21	23	25	26	27

The results clearly illustrates that DWC is more advantageous in terms of energy efficiency when feed mixture consists of large amount of middle boiling component as compare to the concentration of light and heavy component in feed stream.

Table 4-7: Analysis of DWC thermal efficiency with variable molar concentration of toluene in feed

No.	Feed Composition (Mole Fraction)	Toluene Concentration (Mole %)	Energy for Conventional System (kW)	Energy for DWC (kW)	Energy Saving %
Case 1	(0.40,0.20,0.40)	20	2048	1571	23
Case 2	(0.35,0.30,0.35)	30	2167	1507	30
Case 3	(0.33,0.33,0.34)	33	2041	1345	34
Case 4	(0.30,0.40,0.30)	40	2130	1341	37
Case 5	(0.25,0.50,0.25)	50	2274	1381	39
Case 6	(0.20,0.60,0.20)	60	2485	1498	39
Case 7	(0.15,0.70,0.15)	70	2438	1444	40
Case 8	(0.20,0.80,0.20)	80	2335	1329	43

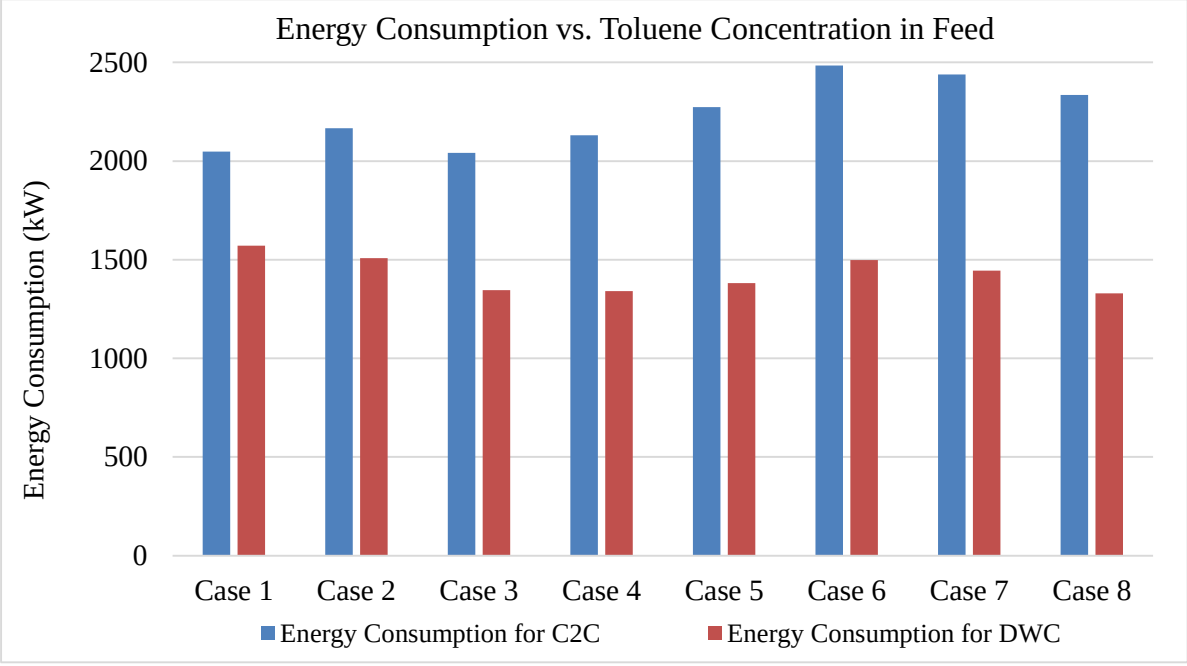


Figure 4-39: Analysis of Energy Saving with Variable Toluene Concentration in Feed

Figure 4-39 shows that energy saving is maximum for case 8 when concentration of toluene in feed is 80%.

4.10 Effect of Side Product Draw and Feed Stage Location on Reboiler Duty

The effect of feed stage and side product draw location on DWC energy consumption is also studied for simulation study of BTE mixture. Figure 4-40 represents the effect of feed tray location on DWC energy consumption. The results shows that minimum energy consumption is 1345 kW when the location of feed stage is 9th tray while the feed stage which is estimated by proposed shortcut design method is also the same 9th tray. It is observed that reboiler duty is insensitive to variation in feed stage location for considerable range. Figure 4-41 represents the effect of side product draw tray location on DWC energy consumption. For variation in side product draw tray location, the minimum reboiler duty arises at 26th tray and shortcut design method also estimate 26th tray as side product draw location.

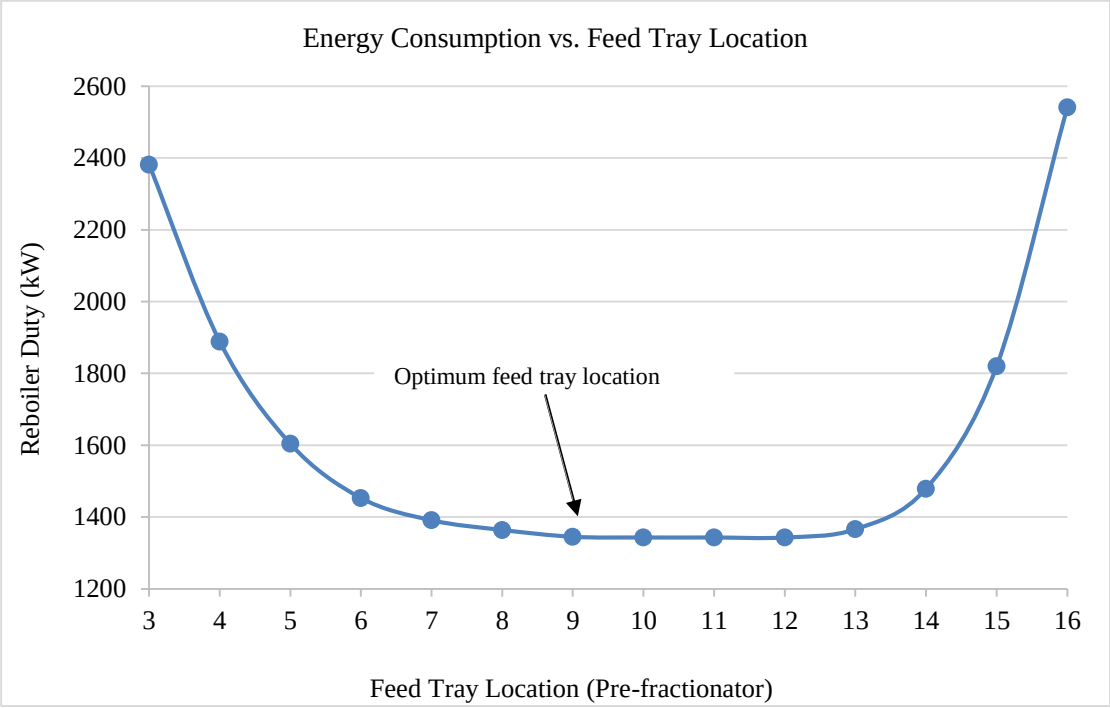


Figure 4-40: Effect of Feed Stage Location on Reboiler Heat Duty

The above two observation illustrates that the proposed shortcut design method is suitable to determine the optimal structure of DWC.

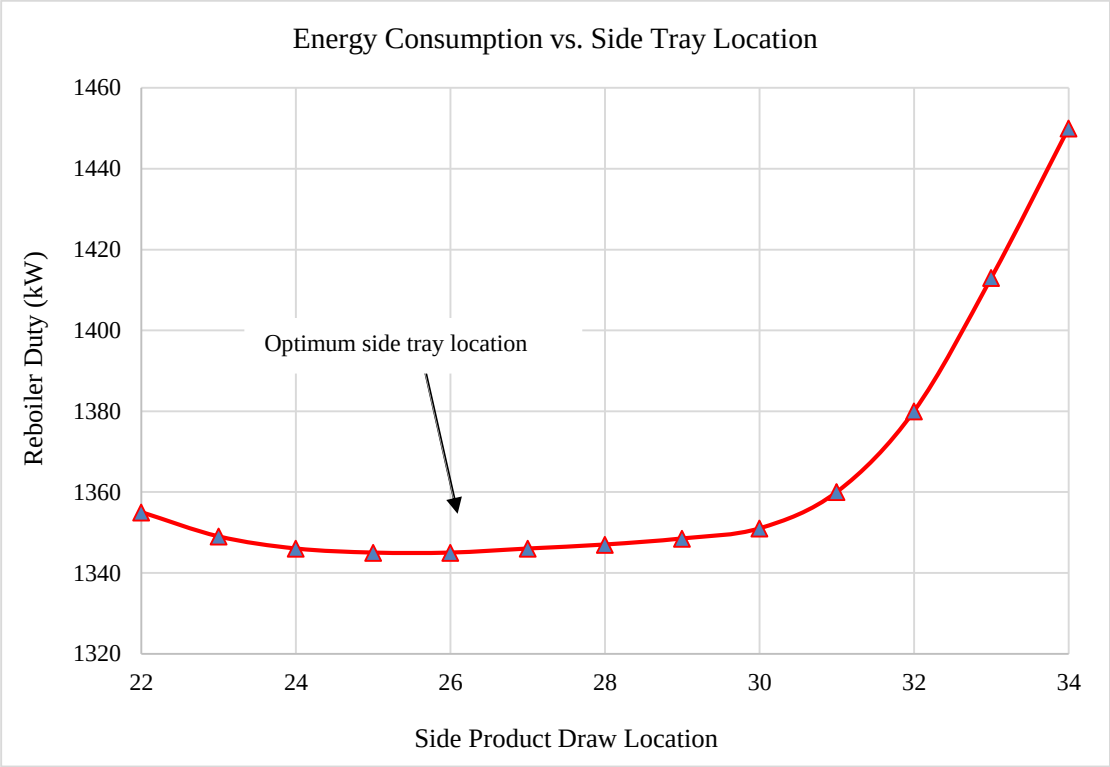


Figure 4-41: Effect of Side Product Draw Location on Reboiler Heat Duty

4.11 Effect of Variable Reflux Ratio on DWC Product Purities

Reflux ratio is very important factor in design and operation of the divided wall column. The study of the influence of reflux ratio on DWC product purity is carried out. Physically, when reflux ratio is increased then more amount of overhead liquid which contains more volatile components is refluxed back to the top of column. Due to more refluxed liquid, the liquid flowrate at top of column increases and then component separation becomes better at top. This effect is studied for BTE mixture. It is observed that as the reflux ratio is increased the product purity of lighter component (benzene) increases and its purity is highest at reflux ratio value of 5.5. The purity of middle component toluene decreases by increasing the reflux ratio, while the purity of heavy

component ethyl-benzene changes hardly by increasing the reflux ratio and there is no any impact of reflux ratio on the purity of the heavy component.

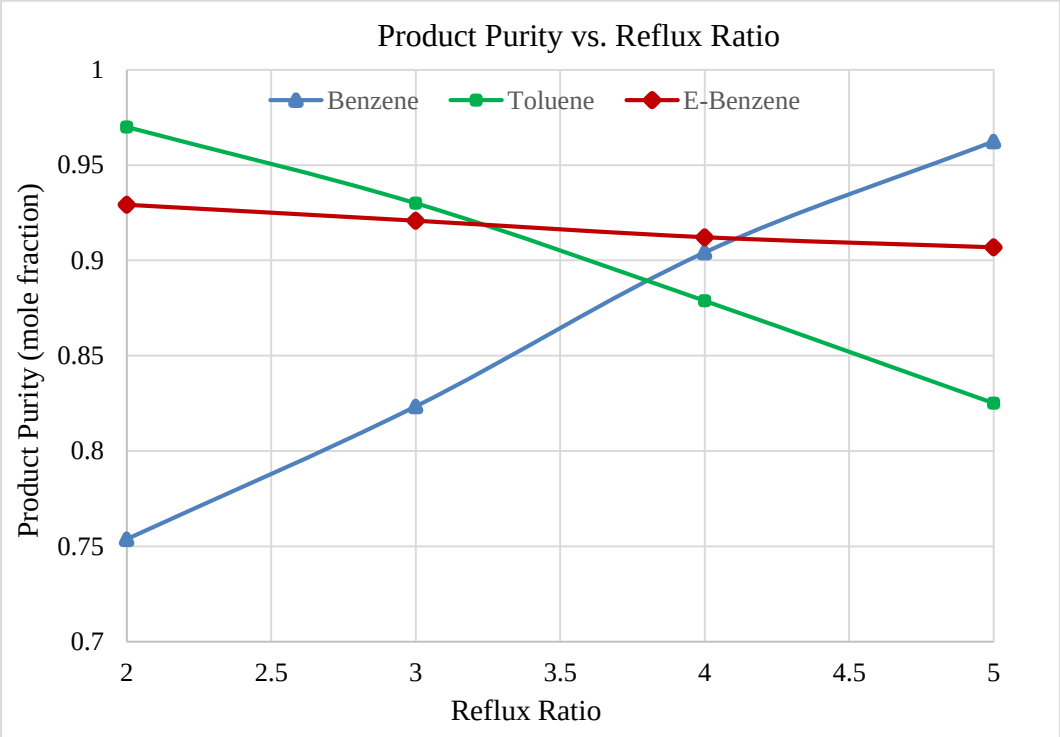


Figure 4-42: Effect of Reflux Ration on DWC Product Purity

4.12 Effect of Variable Feed Tray Location on DWC Product Purities

Optimal feed stage location selection also plays a significant role in the DWC operation. In general, when feed is entered at a tray near the top of the column, then most of the volatile component along with middle component will move towards the top of column and then the bottom product will be free from traces of light component. It is observed that, feed tray location has not any considerable effect on the product purities of all the three components. There is a very minor variation in the composition of toluene and ethyl-benzene, while the composition of the benzene almost remains the same.

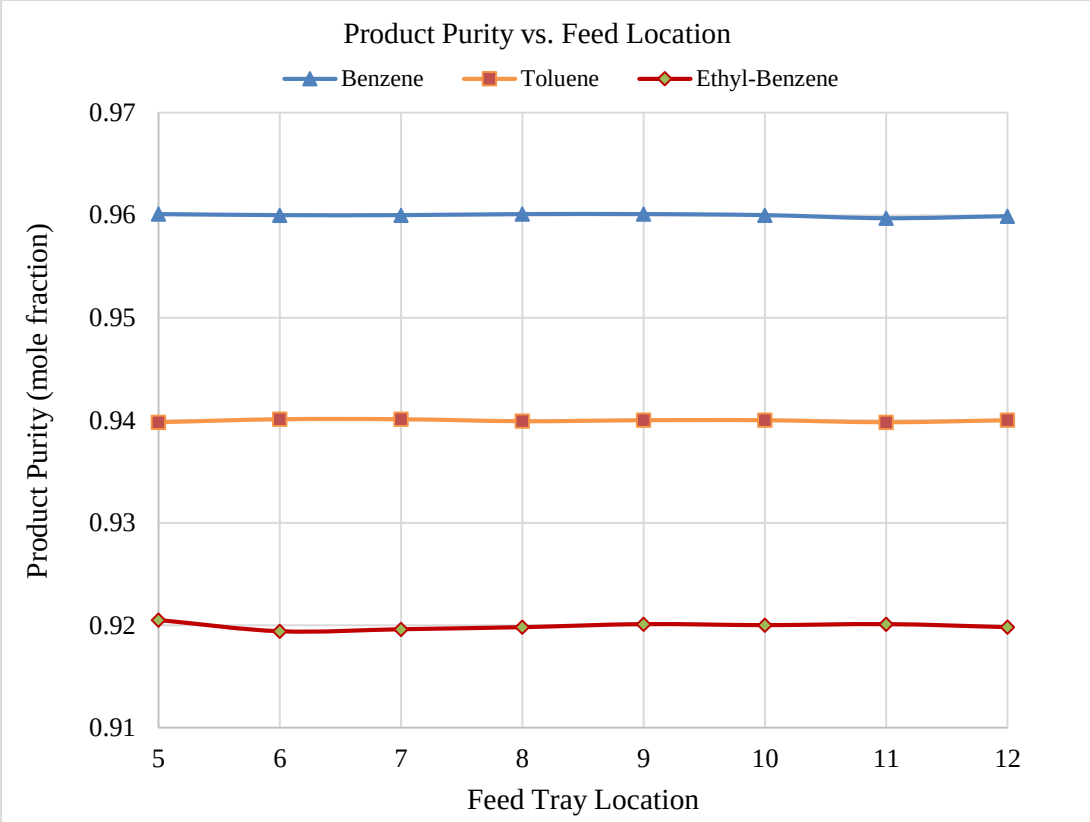


Figure 4-43: Effect of Feed Stage Location on DWC Product Purity

4.13 Effect of Variable Reboiler Duty on DWC Product Purities

Reboiler duty is the amount of energy which is consumed in the separation of the feed components. The value of the reboiler duty for the case study of the BTE mixture is increased in the range of 1300 kW-1700 kW and the effects are investigated on the product purities of all three components. It is observed that by increasing the reboiler duty the purities of all components increased because separation becomes better by increasing the amount of energy required for proper separation.

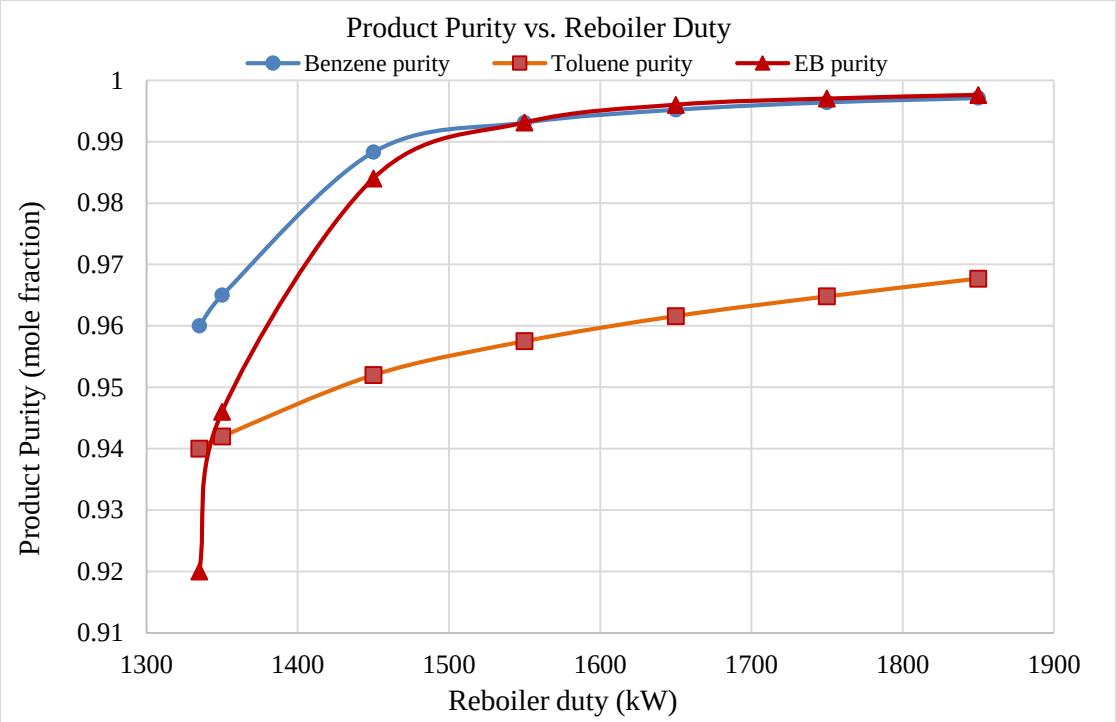


Figure 4-44: Effect of Variable Reboiler Duty on DWC Product Purity

4.14 Effect of Available Energy on Profitability of Process

Sometimes for any case study, if the available energy is greater than the optimal energy required for optimal operation of DWC due to some reason then the product purity of the components will be increased. This excess energy could be used to further purify the separating components. In this situation, one could analyze the current scenario regarding which product is the most costly and which is the cheapest. Normally the lighter products are cheaper than the heavier components, so in such a case, one should focus on the purities of middle and heavy components and try to get the maximum profit by utilizing the available energy that is greater than optimal energy.

4.15 Optimization Results for other Case Studies

The energy consumption in the DWC is mainly dependent on internal liquid and vapor flow distribution. In this section, optimization results for BTX, BTE and alkanes application are presented in graphical form.

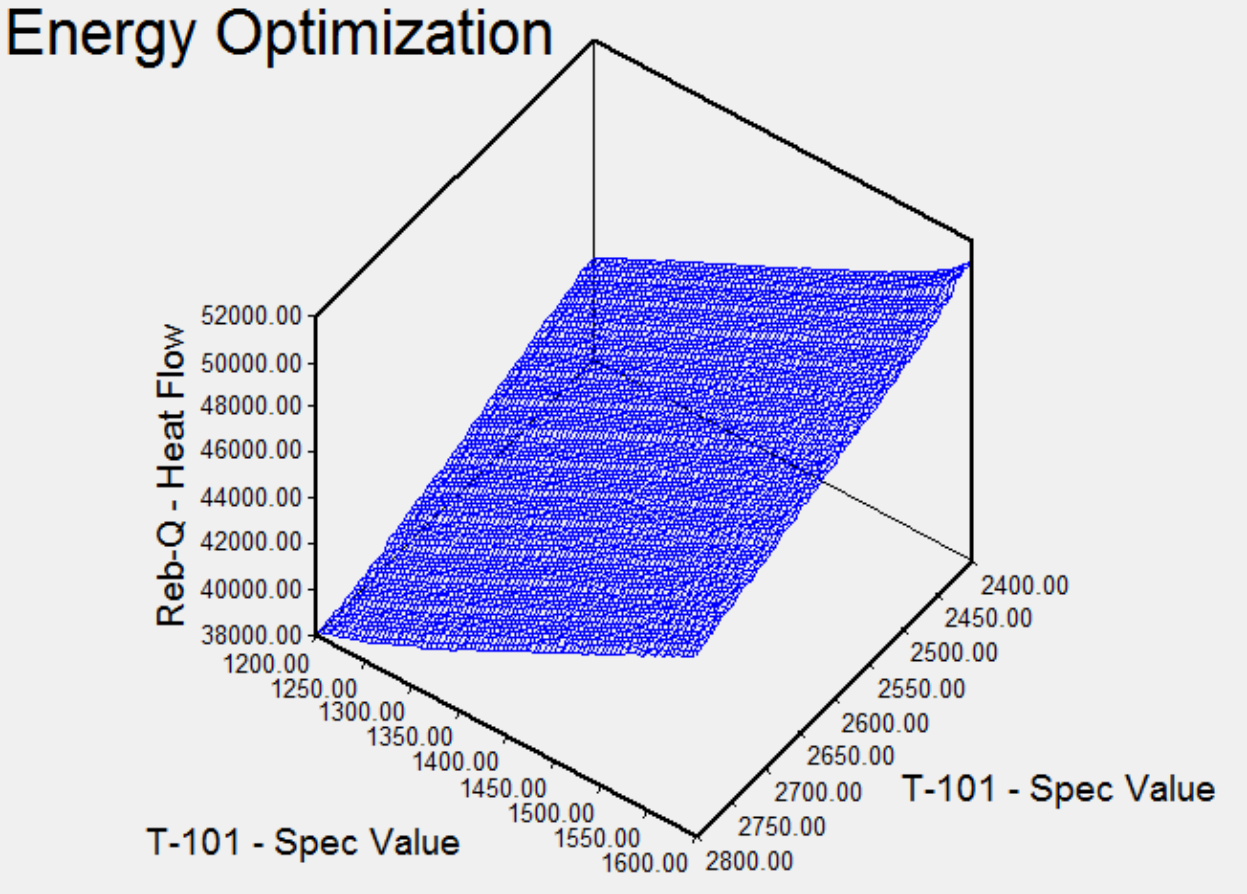


Figure 4-45: Internal Flow Distribution Effect on DWC Reboiler Duty: BTX Separation

For BTX application, the minimum energy consumption after optimization is 44110 kW when internal liquid and vapor flow distribution are 1375 kmol/h and 2550 kmol/h respectively. For BTE mixture application, the minimum energy consumption after optimization is 1345 kW when internal liquid and vapor flow distribution are 58 kmol/h and 107 kmol/h respectively. For alkanes application, the minimum energy consumption is 472 kW and the optimal internal liquid and vapor flow rate are 18 kmol/h and 35 kmol/h. Any variation in internal flow distribution from optimal conditions could results in a sensitive and asymmetrical effect on separation efficiency and energy efficiency.

Simulation results of conventional two-column system for all selected case studies are presented in Figure 4-48 to Figure 4-51 along with technical data sheets.

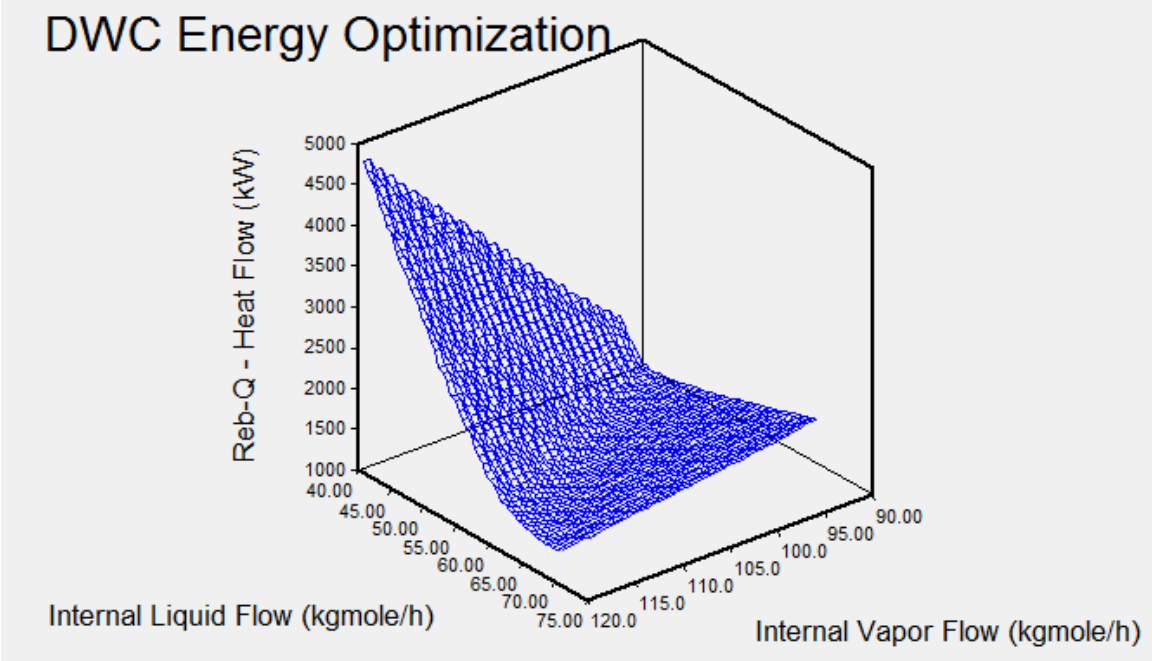


Figure 4-46: Internal Flow Distribution Effect on DWC Reboiler Duty: BTE Separation

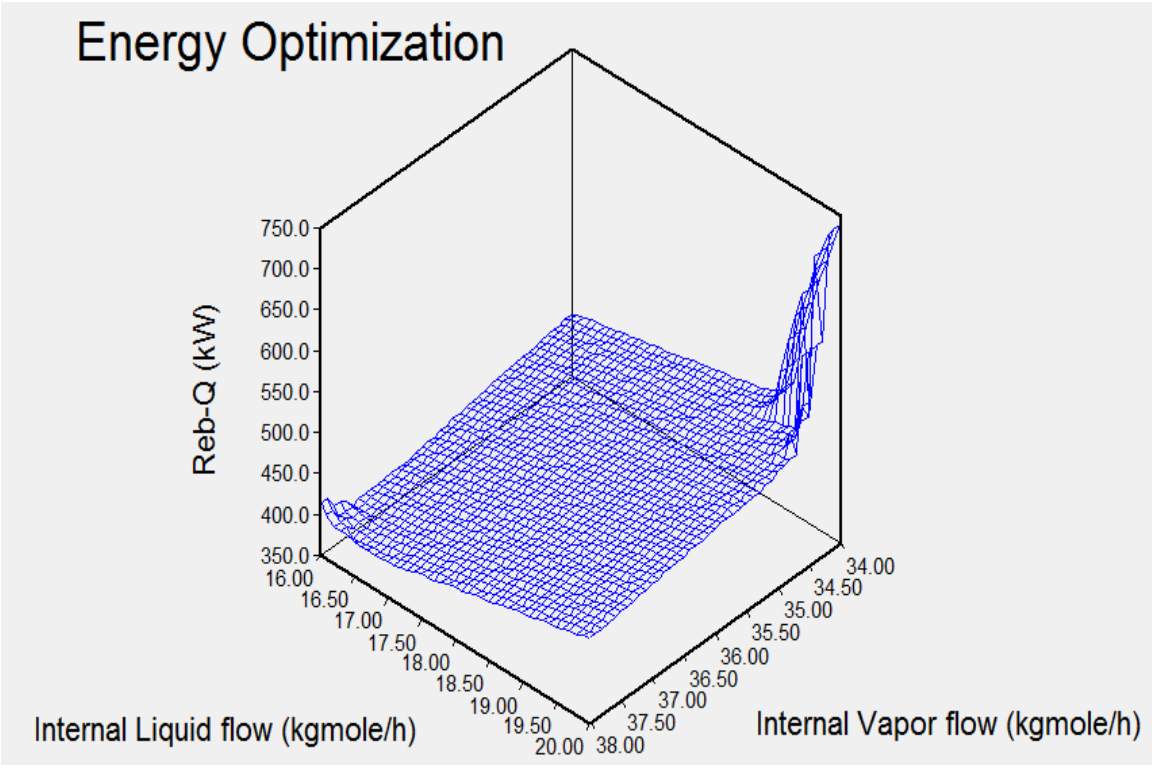
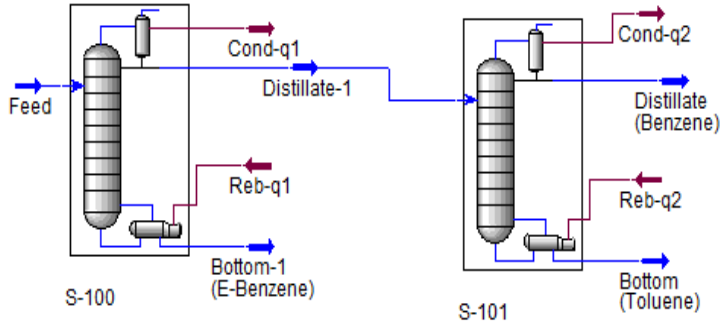


Figure 4-47: Internal Flow Distribution Effect on DWC Reboiler Duty: Alkanes Separation

Feed		
Temperature	128.3	C
Pressure	200.0	kPa
Molar Flow	100.0	kgmole/h
Master Comp Mole Frac (Benzene)	0.3300	
Master Comp Mole Frac (Toluene)	0.3300	
Master Comp Mole Frac (E-Benzene)	0.3400	

Distillate-1		
Temperature	110.9	C
Pressure	170.0	kPa
Molar Flow	65.26	kgmole/h
Master Comp Mole Frac (Benzene)	0.5057	
Master Comp Mole Frac (Toluene)	0.4844	
Master Comp Mole Frac (E-Benzene)	0.0099	

Distillate (Benzene)		
Temperature	96.07	C
Pressure	160.0	kPa
Molar Flow	32.50	kgmole/h
Master Comp Mole Frac (Benzene)	0.9950	
Master Comp Mole Frac (Toluene)	0.0050	
Master Comp Mole Frac (E-Benzene)	0.0000	



Bottom (Toluene)		
Temperature	135.7	C
Pressure	200.0	kPa
Molar Flow	32.76	kgmole/h
Master Comp Mole Frac (Benzene)	0.0202	
Master Comp Mole Frac (Toluene)	0.9600	
Master Comp Mole Frac (E-Benzene)	0.0198	

S-100		
Number of Trays	27.00	
Top Stage Press	170.0	kPa
Duties Summary (Condenser)	-1373	kW
Reboiler Duty	1397	kW
Reflux Ratio	1.381	

S-101		
Number of Trays	27.00	
Top Stage Press	160.0	kPa
Duties Summary (Condenser)	-811.6	kW
Reboiler Duty	832.8	kW
Reflux Ratio	2.019	

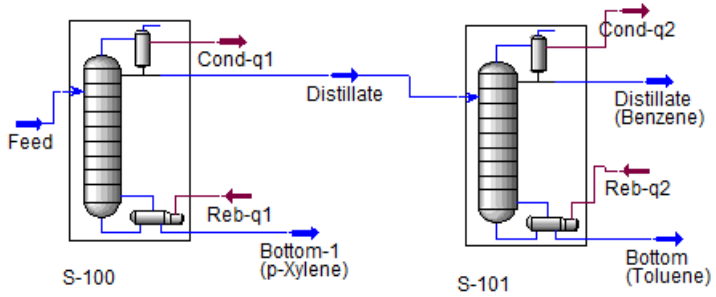
Bottom-1 (E-Benzene)		
Temperature	164.1	C
Pressure	210.0	kPa
Molar Flow	34.74	kgmole/h
Master Comp Mole Frac (Benzene)	0.0000	
Master Comp Mole Frac (Toluene)	0.0400	
Master Comp Mole Frac (E-Benzene)	0.9600	

Figure 4-48: Flow Sheet of Conventional Column Scheme: BTE Application

Feed		
Temperature	71.72	C
Pressure	37.00	kPa
Molar Flow	3600	kgmole/h
Master Comp Mole Frac (Benzene)	0.3000	
Master Comp Mole Frac (Toluene)	0.3000	
Master Comp Mole Frac (p-Xylene)	0.4000	

Distillate		
Temperature	54.89	C
Pressure	30.00	kPa
Molar Flow	2148	kgmole/h
Master Comp Mole Frac (Benzene)	0.5029	
Master Comp Mole Frac (Toluene)	0.4961	
Master Comp Mole Frac (p-Xylene)	0.0010	

Distillate (Benzene)		
Temperature	40.15	C
Pressure	25.00	kPa
Molar Flow	1077	kgmole/h
Master Comp Mole Frac (Benzene)	0.9900	
Master Comp Mole Frac (Toluene)	0.0100	
Master Comp Mole Frac (p-Xylene)	0.0000	



Bottom (Toluene)		
Temperature	75.82	C
Pressure	35.00	kPa
Molar Flow	1071	kgmole/h
Master Comp Mole Frac (Benzene)	0.0129	
Master Comp Mole Frac (Toluene)	0.9850	
Master Comp Mole Frac (p-Xylene)	0.0021	

S-100		
Number of Trays	29.00	
Duties Summary (Condenser)	-4.097e+004	kW
Reflux Ratio	1.001	
Reboiler Duty	4.229e+004	kW

S-101		
Number of Trays	22.00	
Duties Summary (Condenser)	-2.171e+004	kW
Reflux Ratio	1.250	
Reboiler Duty	2.212e+004	kW

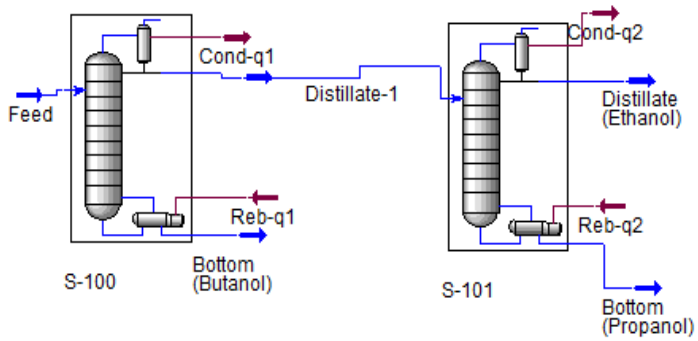
Bottom-1 (p-Xylene)		
Temperature	107.0	C
Pressure	40.00	kPa
Molar Flow	1452	kgmole/h
Master Comp Mole Frac (Benzene)	0.0000	
Master Comp Mole Frac (Toluene)	0.0100	
Master Comp Mole Frac (p-Xylene)	0.9900	

Figure 4-49: Flow Sheet of Conventional Column Scheme: BTX Application

S-101		
Number of Trays	27.00	
Duties Summary (Condenser)	-1128	kW
Reflux Ratio	4.305	
Reboiler Duty	1144	kW

S-100		
Number of Trays	32.00	
Duties Summary (Condenser)	-1873	kW
Reflux Ratio	1.010	
Reboiler Duty	1876	kW

Distillate (Ethanol)		
Temperature	72.44	C
Pressure	80.00	kPa
Molar Flow	19.59	kgmole/h
Master Comp Mole Frac (Ethanol)	0.9900	
Master Comp Mole Frac (1-Propanol)	0.0100	
Master Comp Mole Frac (1-Butanol)	0.0000	



Bottom (Propanol)		
Temperature	96.59	C
Pressure	100.0	kPa
Molar Flow	60.71	kgmole/h
Master Comp Mole Frac (Ethanol)	0.0099	
Master Comp Mole Frac (1-Propanol)	0.9850	
Master Comp Mole Frac (1-Butanol)	0.0051	

Feed		
Temperature	93.95	C
Pressure	100.0	kPa
Molar Flow	100.0	kgmole/h
Master Comp Mole Frac (Ethanol)	0.2000	
Master Comp Mole Frac (1-Propanol)	0.6000	
Master Comp Mole Frac (1-Butanol)	0.2000	

Distillate-1		
Temperature	87.54	C
Pressure	90.00	kPa
Molar Flow	80.30	kgmole/h
Master Comp Mole Frac (Ethanol)	0.2491	
Master Comp Mole Frac (1-Propanol)	0.7471	
Master Comp Mole Frac (1-Butanol)	0.0038	

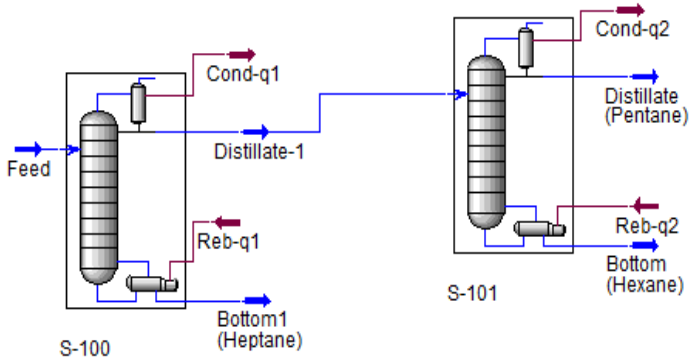
Bottom (Butanol)		
Temperature	118.9	C
Pressure	105.0	kPa
Molar Flow	19.70	kgmole/h
Master Comp Mole Frac (Ethanol)	0.0000	
Master Comp Mole Frac (1-Propanol)	0.0004	
Master Comp Mole Frac (1-Butanol)	0.9996	

Figure 4-50: Flow Sheet of Conventional Column Scheme: Alcohol Application

Feed		
Temperature	70.45	C
Pressure	149.0	kPa
Molar Flow	45.00	kgmole/h
Master Comp Mole Frac (n-Pentane)	0.4000	
Master Comp Mole Frac (n-Hexane)	0.2000	
Master Comp Mole Frac (n-Heptane)	0.4000	

Distillate-1		
Temperature	51.75	C
Pressure	130.0	kPa
Molar Flow	26.86	kgmole/h
Master Comp Mole Frac (n-Pentane)	0.6701	
Master Comp Mole Frac (n-Hexane)	0.3283	
Master Comp Mole Frac (n-Heptane)	0.0016	

Distillate (Pentane)		
Temperature	41.51	C
Pressure	120.0	kPa
Molar Flow	18.09	kgmole/h
Master Comp Mole Frac (n-Pentane)	0.9900	
Master Comp Mole Frac (n-Hexane)	0.0100	
Master Comp Mole Frac (n-Heptane)	0.0000	



Bottom (Hexane)		
Temperature	79.30	C
Pressure	140.0	kPa
Molar Flow	8.769	kgmole/h
Master Comp Mole Frac (n-Pentane)	0.0101	
Master Comp Mole Frac (n-Hexane)	0.9850	
Master Comp Mole Frac (n-Heptane)	0.0049	

S-100		
Number of Trays	29.00	
Duties Summary (Condenser)	-422.0	kW
Reflux Ratio	1.042	
Reboiler Duty	447.8	kW
Top Stage Press	130.0	kPa

S-101		
Number of Trays	23.00	
Duties Summary (Condenser)	-252.0	kW
Reflux Ratio	0.9498	
Reboiler Duty	257.0	kW
Top Stage Press	120.0	kPa

Bottom1 (Heptane)		
Temperature	112.0	C
Pressure	150.0	kPa
Molar Flow	18.14	kgmole/h
Master Comp Mole Frac (n-Pentane)	0.0000	
Master Comp Mole Frac (n-Hexane)	0.0100	
Master Comp Mole Frac (n-Heptane)	0.9900	

Figure 4-51: Flow Sheet of Conventional Column Scheme: Alkanes Application

CHAPTER 5

ECONOMIC EVALUATION OF DWC

An estimate of the overall equipment sizing could be made as once the optimization of DWC has been completed. Economic evaluation are implemented at many levels, with the range from initial rough estimation to reasonable accurate estimation required to obtain the money to purchase the equipment and construction of plant. This sizing calculation is necessary to make an estimate of total capital cost of the project. At final stages of the project, accuracy in the estimates of equipment and energy cost is required, but the effectiveness of process is mainly dependent on the performance of the marketing department who is responsible to give the estimates of raw material cost and products selling price. Unfortunately, the estimates provided by the marketing department are not reliable, hence various simple economic evaluation procedures are used.

5.1 Equipment Sizing

All the equipment used in the required process should be properly sized. The size (length, diameter) of the equipment is dependent on the amount of flow rates passed through it. The technical data needed for equipment sizing could be taken from DWC optimization data.

5.1.1 Diameter of Column Shell

The simulation results for the optimized DWC from HYSYS will be used for column shell sizing. Suitable mathematical correlations are available to calculate this maximum vapor

velocity. To determine the column diameter, equations from Sinnot [96] are used. In this study the actual vapor velocity (U_{act}) is 85% of the maximum vapor velocity.

$$U_{max} = (-0.171{l_t}^2 + 0.27l_t - 0.047)\sqrt{\frac{\rho_L - \rho_v}{\rho_v}} \quad (5.\ 1)$$

In this equation, l_t is tray spacing between any two consecutive trays. Tray spacing chosen for this study is 0.6 m and this value is chosen to be enough for the easy maintenance and cleaning of the column. ρ_L and ρ_V are the liquid and vapor density in kg/m^3 and it is assumed that the flow is constant. The column diameter D is calculated using equation.

$$D = \sqrt{\frac{4G}{(\pi U_{act}\rho_v)}} \quad (5.\ 2)$$

U_{act} is the actual vapor velocity in m/s. By retrieving values of volumetric vapor flow rate and vapor density from HYSYS and multiplying these two values, the vapor mass flow rate G could be determined in kg/s.

The other internals that are feed distributor, down comers and vapor/liquid draw-off pipes are not considered here because their cost is negligible as compare to the column and trays. The DWC always would be sized to hold maximum liquid and vapor flow rate in all the three sections, these maximum flow rates are available from rigorous simulation of the DWC.

5.1.2 Column height

The column height could be easily estimated when the number of column stages are known. The column height H could be calculated by multiplying the actual number of stages with the spacing between the trays and adding some more space as an additional space.

Normally, some additional space is required at the top of the column as disengaging space for vapor and liquid or for the entrance of the reflux piping. Similarly, some additional space is also needed at the bottom to maintain the level of the liquid in the base to provide the required net positive suction head (NPSH) for the liquid pump. It is observed that it is design heuristic to add 20% extra height than only for trays to accommodate the liquid sump and vapor disengagement. The height of the column could be calculated from the following relation.

$$H = 1.2 \times N \times l_t \qquad (5.3)$$

Where N is the actual amount of column stages and l_t is the spacing (0.6m) between any two trays. Volume of the column could be determined by multiplying the cross-section area of the column with the height.

5.1.3 Tray Spacing

The overall column height depends upon the tray spacingl_t. Normally used tray spacing is from 0.15 m (6 in) to 1 m (36 in) [96]. Tray spacing is small for a small diameter column and for columns with diameter more than 1 m, this value is between 0.25-0.6 m [97]. The tray spacing should be sufficient enough to accommodate the feed and product streams arrangements and for manways to clean the trays etc.

5.1.4 Heat Exchangers Sizing

In present study, condenser and reboiler are considered as shell and tube heat exchanger which are the mostly used heat exchangers in the industries. Plate type heat exchangers could also be used if fouling is not a serious problem as these heat exchanger offer greater heat exchanger area. The raw water is utilized to cool down the hot medium in condenser

and steam is used for heating the cold medium in reboiler. The area of the heat transfer for heat exchanger is required to estimate the cost of the exchanger. The heat transfer area of condenser and reboiler could be found based on the overall heat transfer coefficients by using the design equation given below.

$$Q = UA\Delta T_{lm} \quad (5.4)$$

Q is the heat duty of the condenser or reboiler that is retrieved directly from HYSYS simulation, A is heat transfer area (m^2), U is value of overall heat transfer coefficient ($W/m^2.^0C$) and ΔT_{lm} is the differential temperature driving force (^0C). Value of U for different heat exchangers are given in Table 5-1.

Table 5-1: Different Values of Heat-Transfer Coefficients

Heat Exchanger Type	Heat Transfer Coefficient	Units
Floating Head	250-750	$W/m^2.^0C$
Kettle Reboiler	500-1000	$W/m^2.^0C$

The value of U is dependent on the liquid and vapor phases on both sides of the heat exchanger. In this study an average of 490 $W/m^2.^0C$ and 1000 $W/m^2.^0C$ is considered for U of the floating head condenser and the kettle reboiler respectively. The differential temperature driving force could be measured by using following equation.

$$\Delta T_{lm} = \frac{(\Delta T_A - \Delta T_B)}{ln\left(\frac{\Delta T_A}{\Delta T_B}\right)} \quad (5.5)$$

ΔT_A and ΔT_B are temperature difference between two different streams on both sides of condenser and reboiler.

5.1.5 Temperature of Condenser Inlet and Outlet Streams

Temperatures (inlet and outlet) of hot stream entering in the condenser is found from the HYSYS flow sheet. The vapor stream at the column top is the hot inlet stream of the condenser and the distillate stream is the cooled outlet stream of the condenser.

In this study the cooling medium temperature difference is considered as 10^0C. The cooling medium temperature in the condenser rise from 30^0C to 40^0C. When cooling medium in condenser is raw water, then the temperature change between inlet and outlet streams of the condenser is usually in range of 7^0C to 10^0C.

5.1.6 Temperature of Reboiler Inlet and Outlet Streams

Temperatures of inlet and outlet streams of reboiler are found from HYSYS flow sheet. The liquid material at the column bottom is the inlet feed of reboiler and hot boil-up stream is the heated outlet stream of the reboiler. The steam is utilized as a heating source in the reboiler. It is supposed that 4 bar steam pressure (low pressure) at temperature of 160^0C is used. The steam inlet temperature is set to 160^0C. The minimum temperature difference (ΔT_{min}) for the reboiler has to be in the range of 20^0C-40^0C. In the present study, the minimum temperature difference (ΔT_{min}) is taken as 35^0C. A heat transfer coefficient (U) for kettle type reboiler is taken as 1000 W/m^2.^{0}C.

5.2 Economic Evaluation of DWC System

5.2.1 Economic Evaluation Assumptions

The economic evaluation of the DWC is based on the following assumptions:

- The divided wall column is a vertical process vessel and the maximum column operating pressure is 10 bar.
- The trays used in the column are sieve trays.
- The condenser used is a floating head heat exchanger and the cooling water is the cooling medium.
- The reboiler used is a kettle type reboiler and steam is the heating medium in the reboiler.
- The construction material used is stainless steel.
- The operating time of the column is 346 days/year and payback period is 3 years.

5.3 Sinnot Cost Method

In Sinnot cost method the purchase cost, C_e, of the vertical column could be calculated by using the following equation [96].

$$C_e = a + bS^n \tag{5. 6}$$

Where n is the exponent for different type of equipment, a and b are the constants, and S is the sizing parameter.

Table 5-2: Cost Data for Different Types of Equipment's

Equipment	a	b	n	Size Parameter
Process vessels	15000	68	0.85	Shell mass (kg)
Sieve trays	110	380	1.8	Diameter (m)
Floating Head Condenser	24000	46	1.3	Area (m^2)
Kettle Reboiler	25000	340	0.9	Area (m^2)

In this cost method, the cost evaluation is done at ambient operating pressure and the construction material used is stainless steel. If the sieve trays, reboiler and condenser construction material is carbon steel then the value of factor n is taken as 1.2. The purchased cost that is calculated by equation 5.6 is multiplied by a factor of 6 to find the total fixed capital cost of equipment. In the same way, capital cost of all the major equipment's (column, trays, condenser and reboiler) could be determined.

5.4 Equipment Cost

In literature, there are two different kinds of capital equipment costs that are bare module cost and installed cost. The bare module cost is only the equipment cost, whereas the installed cost is the cost of equipment including its installation cost in the plant, e.g. instrumentation, electrical and civil, paint, insulation and manpower. The total capital investment in a complete plant is about four to five times the major equipment cost. In this study, the cost correlations for the cost evaluation of column including reboiler, condenser and trays are used from Douglas [97], Turton et al. [98] and Kiss [99]. Cost evaluation comprises of calculating operating and capital costs of DWC for ternary feed system. Cost correlations used for economic evaluation of any distillation system would be updated with latest cost index. Marshal and Swift equipment cost index (M & S) is used with value of 1536. All estimated costs are presented in US dollars.

5.4.1. Column Vessel

The value of purchase cost and installed cost of the distillation column vessel with carbon steel as construction material is given by the following mathematical correlations which are taken from Kiss [99].

$$Purchased\ Cost\ (\$) = \left(\frac{M\ \&\ S}{280}\right)(957.9D^{1.066}H^{0.802}F_C) \quad (5.\ 7)$$

$$Installed\ Cost\ (\$) = \left(\frac{M\ \&\ S}{280}\right)(957.9D^{1.066}H^{0.802})(2.18 + F_C) \quad (5.\ 8)$$

In above equation, D is the distillation column diameter and H is the the vertical process vessel height and both are expressed in meters.

Table 5-3: Material Factors for Different Process Vessels

	Material of Shell			
Factor	Stainless Steel	Carbon Steel	Titanium	Monel
F_m Clad	2.25	1	4.25	3.89
F_m Solid	3.67	1	7.89	6.34

The cost factor (F_C) is given below and the pressure used is in bar.

$$F_C = F_m F_P \quad (5.\ 9)$$

$$F_P = 1 + 0.0074(P - 3.48) + 0.00023(P - 3.48)^2 \quad (5.\ 10)$$

As the operating pressure of the equipment increases the thickness of the equipment wall also increases. So a pressure factor of equipment is dependent on its wall thickness. For a cylindrical process (pressurized) vessel that is operating at more pressure than the ambient pressure, the correlation between the wall thickness and the design pressure needed to bear the stress in cylindrical section of column is presented as

$$t = \frac{PD}{2SE - 1.2P} + CA \quad (5.\ 11)$$

In given equation above, P is design pressure (bar), t is thickness of wall (m), S is maximum permissible stress of material (bar), D is vessel diameter (m), E is welding efficiency and CA is corrosion allowance (m). The typical values of corrosion allowance

are from 3.15-6.3 mm (0.125-0.25 inches) and values for welding efficiency are from 1.0 to 0.6 [98].

5.4.2. Column Sieve Trays

The cost of the sieve trays depends upon the cross-section area. The cross-section area of the sieve trays could be found by using the given equation:

$$A = \frac{\pi D^2}{4} \tag{5. 12}$$

The installed cost of sieve trays is determined by using the equation:

$$Installed\ Cost\ (\$) = \left(\frac{M\&S}{280}\right) \times 97.2D^{1.55} \times H \times F_C \tag{5. 13}$$

For standard tray spacing ($l_t = 0.6m$) the correction factor is given as follows:

$$F_C = F_t + F_m \tag{5. 14}$$

For sieve trays, F_t (tray factor) is 0, for bubble cap trays it is 1.8 and for complex trays it is 3. For stainless steel, F_m (material factor) is 1.7, for carbon steel it is 1.0 and for higher alloys its value is high.

5.4.3. Heat Exchangers (Condenser & Reboiler)

The heat exchanger cost depends upon cross-section area. The heat exchanger installed cost is calculated as follows:

$$Purchased\ Cost\ (\$) = (\frac{M\&S}{280})(474.7 \times A^{0.65} \times F_C) \tag{5. 15}$$

$$Installed\ Cost\ (\$) = (\frac{M\&S}{280})(474.7 \times A^{0.65})(2.29 + F_C) \tag{5. 16}$$

Area of heat exchanger (A) is given in m^2 and the above relations are valid only upto size of $20 < A < 500\ m^2$. The cost factor (F_C) is determined as:

$$F_C = F_m(F_d + F_P) \quad (5.\ 17)$$

Where F_d is the design factor of the heat exchangers, F_P and F_m are the pressure factor and material factor of the shell and tube heat exchangers and values are given in Table 5-4 [99].

Table 5-4: Material, Pressure and Design Factors for Different Heat Exchangers

Material of Shell/tubes	F_m	Design Type	F_d	Design Pressure (bar)	F_P
CS/SS	2.81	Kettle type Reboiler	1.34	<10	0
CS/CS	1.0	Floating Head	1.0	25	0.1
CS/Brass	1.3	U-tube	0.85	35	0.25
CS/Monel	2.15	Fixed-tube sheet	0.8	65	0.52
SS/SS	3.75	-	-	>70	0.55
CS/Titanium	8.95	-	-	-	-

5.4.4. Effect of Time on Cost

The installed cost calculated above is not the cost for the present time. It is essential to update the cost correlations to take changes in economic inflation into account. The above calculated cost have to be converted into the capital cost for the present time. This can be done by using the following equation:

$$C_2 = C_1 \frac{I_2}{I_1} \quad (5.\ 18)$$

In above equation, C_1 is the cost of the time (base time) when cost is known, C_2 is the cost for the present time, I_1 and I_2 are the cost index for base time and present time respectively. Chemical industries uses different cost indices to modify and estimate the inflation effects. In these indices, Marshall and Swift Process Industry Index, Chemical Engineering Plant Cost Index and Nelson-Farrar Refinery Construction Index are included.

5.5 Estimation of Operating (utility) Costs

Typical process utilities are cooling water, process steam, compressed air, electricity, heated water, process water, and refrigerants etc. In any distillation system reboilers and condensers are required for the process and these heat exchangers constitutes the major source of energy consumption in distillation process in the form of cooling and heating. Operating costs of the distillation system mainly consists of these two utility costs. Unlike total capital and labor related expenses, operating cost could not be directly correlate with inflationary indexes because utility costs are not dependent on capital cost and labor cost and these utility costs changes unpredictably. Normally, utility cost is interlinked with two different variables that are energy cost and inflation. Chemical Engineering Plant Cost Index (CEPCI) represents the inflation rate. Energy costs of cooling water and steam vary rapidly, therefore Ulrich [100] chose two-factor utility cost equation as follows:

$$C_{S,utility} = a \times (CEPCI) + b \times (C_{S,f}) \qquad (5.\ 19)$$

$C_{S,utility}$ is the utility price, $C_{S,fuel}$ is the fuel price in \$/GJ, a and b are utility cost coefficients and CEPCI is an inflation constraint for the projects. The comprehensive information about utility cost coefficients along with examples are given by Ulrich [100].

Table 5-5: Utility Cost Coefficients

Cooling Water, \$/m^3		(0.02< q <12 m^3/s)
	a	b
	$0.0001 + 3.0 \times 10^{-5}\ q^{-1}$	0.0032
Process Steam, \$/kg		(5 < p < 45 barg; 0.05 < m_s< 45 kg/s)
	a	b
	$2.7 \times 10^{-5}\ m_s^{-0.85}$	$0.0034p^{0.05}$

Utility cost coefficients a and b for cooling water and steam are given in Table 5-5 where q is the total water capacity in m^3/s and m_S is total steam capacity of boiler in kg/s. The value used for q is 10 m^3/s because the standard cooling systems are limited to 10 m^3/s and the value used for m_S is 40 kg/s which is the steam flow rate for total steam consumption at plant [100]. The energy cost is also dependent on heat source temperature or heat sink temperature. The following estimated energy costs could be used only for guidelines because actual estimates depends upon the local availability of the utilities. The cooling water cost per year can be determined as follows

$$Cost\ of\ cooling\ water, \frac{\$}{yr} = \left(\frac{kg\ water}{hr}\right) \times \left(\frac{cost,\$}{kg}\right) \times \left(\frac{operating\ Hour}{yr}\right) \quad (5.\ 20)$$

In case of a reboiler, process steam is condensed from saturated vapor or superheated vapor to saturated liquid. The steam cost per year can be calculated as follows

$$Cost\ of\ steam\ , \frac{\$}{yr} = \left(\frac{steam\ cost,\$}{kg\ steam}\right) \times \left(\frac{kg\ steam}{hr}\right) \times \left(\frac{operating\ Hour}{yr}\right) \quad (5.\ 21)$$

5.6 Total Annual Cost

Total annual cost comprised of total capital cost per year and energy cost per year. Total capital cost is the summation of the installed cost for all equipment of DWC. The total annual cost (TAC) could be determined by using the correlation which is taken from Luyben [101].

$$\text{Total Annual Cost (TAC)} = \frac{\text{Total capital cost}}{Payback\ period} + \text{Total operating cost per year} \quad (5.\ 22)$$

5.7 Results and Discussion

In this chapter, a detailed procedure of economic evaluation of column vessel, sieve trays, reboiler and condenser is described. The economic evaluation of all case studies that have been chosen for DWC design are carried out by using Excel program. The results of this evaluation for alcohol application has been presented in tables given below. The economic evaluation of the DWC and conventional distillation column are presented in Table 5-6 and Table 5-7 respectively. The comparison of DWC and conventional distillation column is given in Table 5-8, the results illustrates that there is a significant difference in energy consumption and capital cost of DWC as compare to conventional two-column system. The energy consumption of the DWC is 36% lesser than the conventional two-column system and total annual cost of DWC is 27% less than conventional two- column system. This attractive savings in energy and annual cost provide a perfect direction to use DWC against conventional two-column system for commissioning of new plants.

Table 5-6: Economic Evaluation of DWC: Alcohol Application

Description	**Divided Wall Column**
Economic Details	
Reboiler Duty (kW)	1927
Condenser Duty (kW)	1909
Total Stages	60
Column Diameter (m)	1.4
Column Height (m)	45
Area of Condenser (m^2)	101.24
Area of Reboiler (m^2)	55.06
Installed Cost	
Column Shell Cost (US$)	922274
Column Trays Cost (US$)	68739
Column Condenser Cost (US$)	267204
Column Reboiler Cost (US$)	214531
Total Installed Cost (US$)	1472748
Utilities Cost	
Unit Cost of Cooling Water (US$/$m^3$)	0.073
Cooling Water Cost (US$/yr)	99343
Unit Cost of Steam (US$/Ton)	17.01
Steam Cost (US$/yr)	486288
Total Operating Cost (US$/yr)	585631
Total Annual Cost (US$/yr)	**1076547**

Table 5-7: Economic Evaluation of Conventional Two-Column System: Alcohol Application

Description	**Conventional Two-Column system (In-Direct sequence)**		
Economic Details	S-100	S-101	Total
Reboiler Duty (kW)	1876	1144	3020
Condenser Duty (kW)	1873	1128	3001
Total Stages	32	27	
Column Diameter (m)	1.4	1.1	
Column Height (m)	22.2	19.2	
Area of Condenser (m^2)	68.33	59.34	
Area of Reboiler (m^2)	53.6	32.69	
Installed Cost			
Column Shell Cost (US$)	522844	359879	
Column Trays Cost (US$)	33911	20181	
Column Condenser Cost (US$)	206948	188816	
Column Reboiler Cost (US$)	210816	152868	
Total Installed Cost (US$)	974519	721744	
Utilities Cost			
Unit Cost of Cooling Water (US$/$m^3$)	0.073	0.073	
Cooling Water Cost (US$/yr)	97469	58700	
Unit Cost of Steam (US$/Ton)	17.01	17.01	
Steam Cost (US$/yr)	473418	288694	
Total Operating Cost (US$/yr)	570887	347394	918281
Total Annual Cost (US$/yr)	895727	587975	**1483702**

Table 5-8: Economics Comparison of DWC and Conventional Column System: Alcohol Application

Description	**Conventional Two-Column system**			**Divided Wall Column**	
Economic Details	S-100	S-101	Total		Saving (%)
Reboiler Duty (kW)	1876	1144	3020	1927	36
Condenser Duty (kW)	1873	1128		1909	
Total Stages	32	27		60	
Column Diameter (m)	1.4	1.1		1.4	
Column Height (m)	22.2	19.2		45	
Area of Condenser (m^2)	68.33	59.34		101.24	
Area of Reboiler (m^2)	53.6	32.69		55.06	
Installed Cost					
Column Shell Cost (US$)	522844	359879		922274	
Column Trays Cost (US$)	33911	20181		68739	
Column Condenser Cost (US$)	206948	188816		267204	
Column Reboiler Cost (US$)	210816	152868		214531	
Total Installed Cost (US$)	974519	721744		1472748	
Utilities Cost					
Unit Cost of Cooling Water (US$/$m^3$)	0.073	0.073		0.073	
Cooling Water Cost (US$/yr)	97469	58700		99343	
Unit Cost of Steam (US$/Ton)	17.01	17.01		17.01	
Steam Cost (US$/yr)	473418	288694		486288	
Total Operating Cost (US$/yr)	570887	347394	918281	585631	36
Total Annual Cost (US$/yr)	895727	587975	**1483702**	**1076547**	27

5.8 Effect of Column Height on Reflux Ratio and Reboiler Duty

The simulation of the Alcohol case study is further carried out to observe the effect of the number of column stages on the reflux ratio as well as on the reboiler duty of the column. The obtained results shows that by increasing the number of stages in the column, the reflux ratio will decrease and by decreasing the number of stages it will increase. The main reason of this trend is that, when the number of stages in the column increase the separation between the components becomes easier due to which the reflux ratio decreases. Similarly when column has less number of stages then separation between the components is difficult and results in a higher reflux ratio. The trend is shown in Figure 5-1.

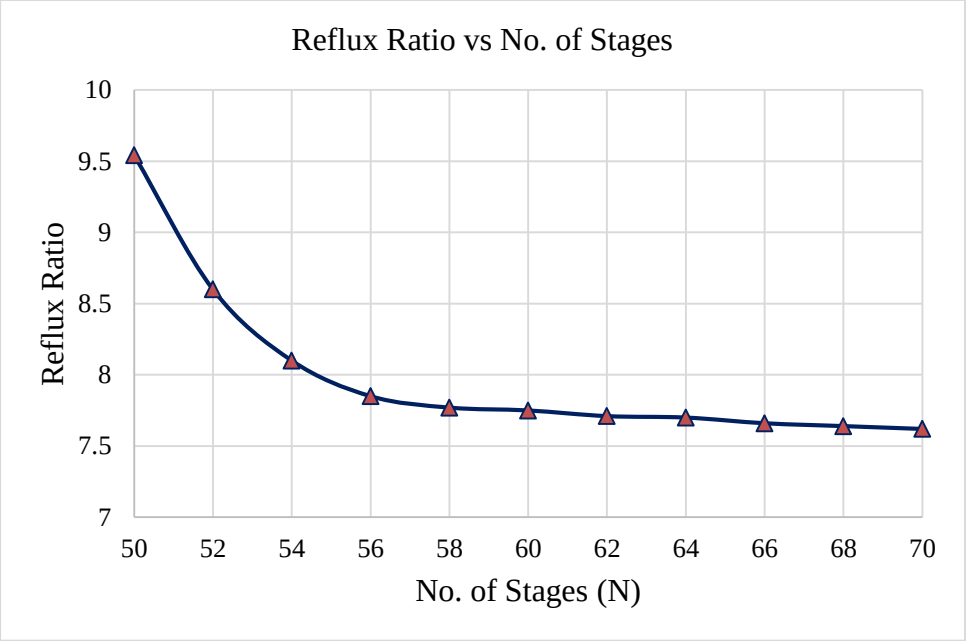


Figure 5-1: Effect of Number of Stages on Reflux Ratio

Similarly in case of reboiler duty, the duty of the column decreases by increasing the number of the stages in the column. Because by increasing the column height the separation becomes much better and less amount of heat input is required to get the required fractionation of the components. When the number of stages in the column are less, then

the more heat input is required to obtain the required separation level of the components. The effect of column height on the reboiler duty is shown in Figure 5-2.

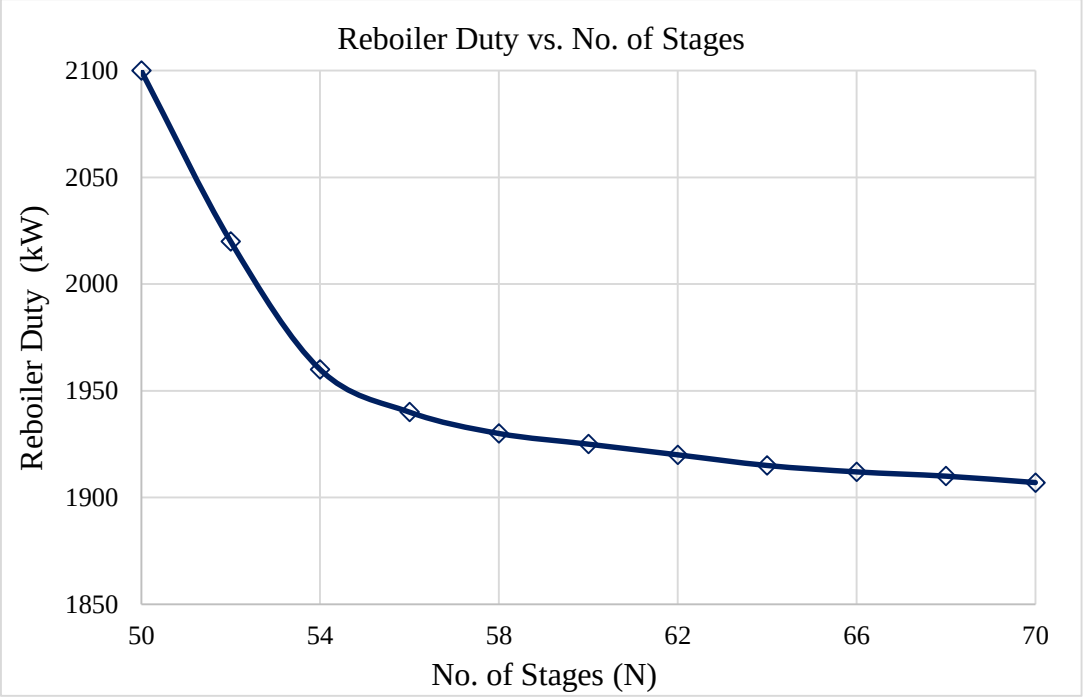


Figure 5-2: Effect of Number of Stages on Reboiler Duty

5.9 Effect of Column Height on Capital Cost and Total Annual Cost

The effect of the column height on the capital cost of column vessel/heat exchanger and total annual cost as well as total operating cost of the DWC is also studied. The effect of column height on capital cost shows that by increasing the column height, the number of stages in column increases but its diameter decreases because the heat exchangers heat input decreased. This effect results in increase in column vessel cost and total annual cost but decrease in heat exchanger cost as well as the total operating cost due to decrease in the heat exchanger area. If the number of stages are decreased then it results in a shorter column and increased reboiler heat input. This reduction in column height causes increase in column diameter and heat exchanger areas. This results in an increase in capital cost as well as total operating cost. These effects are presented in Figure 5-3 and 5-4.

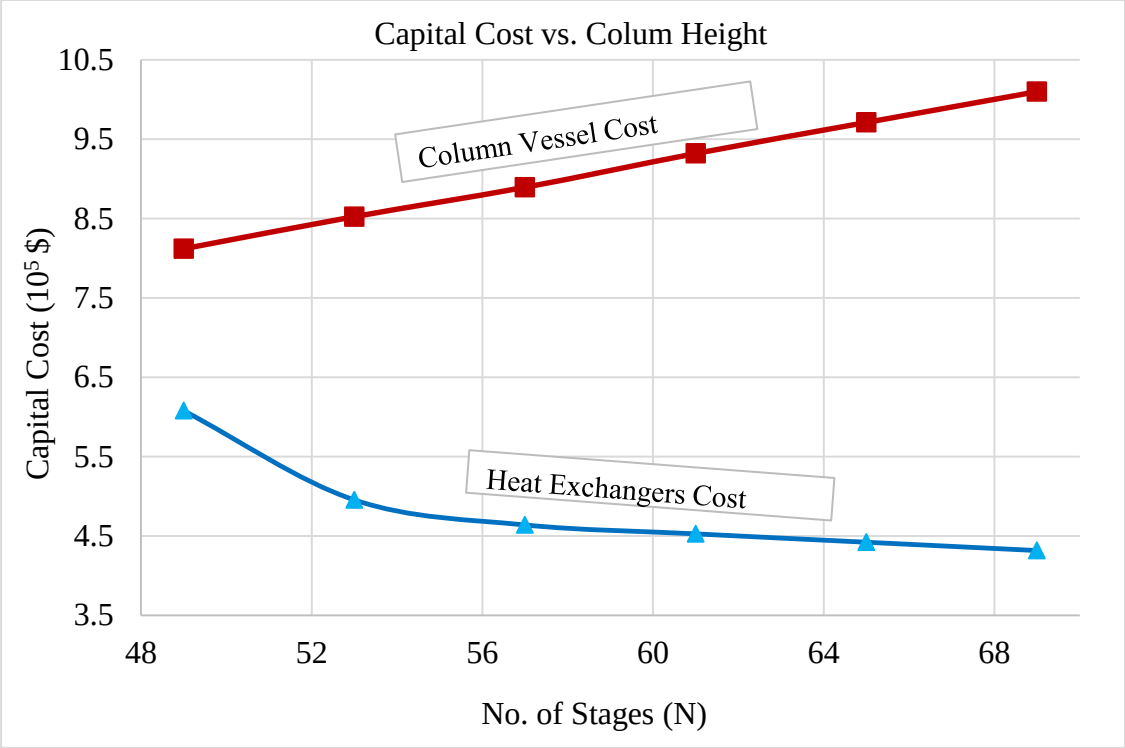


Figure 5-3: Effect of Number of Stages on Capital Cost

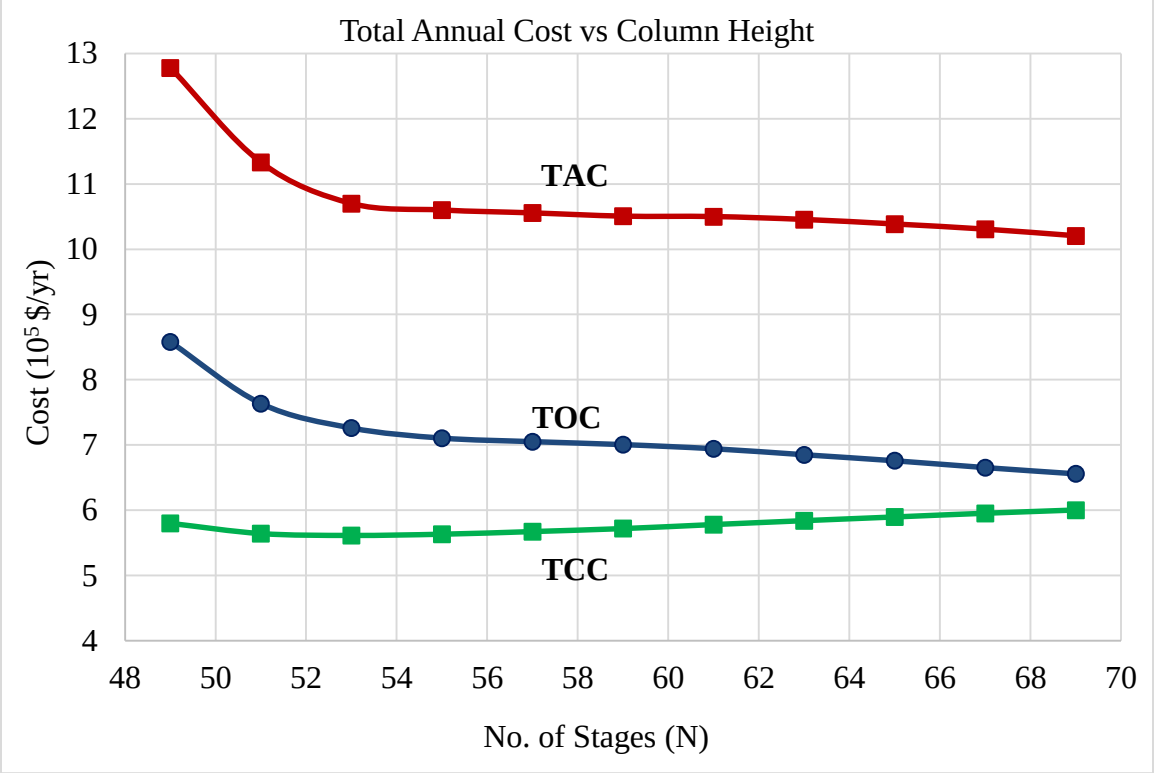


Figure 5-4: Effect of Column Height on Total Annual Cost

CHAPTER 6

RETROFITTING

Currently, process intensification is taken as the key trend to enhance the process effectiveness and the main approach to this intensification is to minimize the equipment's that are being used in the plant. For distillation process, thermal coupling system offers such a method to retrofit the conventional distillation system by the elimination of the reboiler and condenser. Retrofitting offers savings in both energy and investment cost and getting more importance. In distillation system, retrofits suggests some modifications in existing columns to minimize the operation cost by improving the plant efficiency in energy consumption [102]. The other benefit of retrofitting is that the equipment which are useless after retrofitting, they could further used any suitable place in the plant in terms of capacity enhancement on the plant.

The objectives of the retrofitting are the maximum savings in energy consumption, the minimum alteration in the existing equipment or plant and the maximum utilization of the existing equipment. Retrofitting also allows a maximum reuse or recycle of the number of existing equipment on the plant. This retrofitting option is also very suitable on the plants where there is a problem of space. By retrofitting, the plot area of the equipment could be reduced. Retrofitting of conventional distillation system to DWC has gained acceptance due to its potential benefits of reduced energy cost and capital cost.

In case of retrofitting of heat exchangers, the comparison of energy consumption is carried out by adding condenser and reboiler duties. These heat duties values could be used only

for rough or preliminary estimation, but for a detailed analysis, the quality of the heating medium (i.e., high, medium or low pressure steam) that is needed for the process must be taken into account. After retrofitting, some equipment could be reused without any modification and some equipment could be reused with modification.

6.1 Retrofitting Analysis of Alcohol Application

Column operating conditions, feed conditions and product specifications for the case study selected for retrofitting is given in Table 4-5.

For this retrofitting study, conventional two-column system for Alcohol application shown in Figure 4-50 is considered as existing column in the plant and its retrofitting is required.. Simulation results of conventional two column system (Figure 4-50) shows that first columns (S-100) has 32 stages and second column (S-101) has 27 stages having diameter 1.4 m and 1.1 m respectively. Height of both columns are 22.2 m and 19.2 m respectively. Heat duties of condenser and reboiler for column S-100 are greater than other column S-101. Figure 4-22 presents the simulation results of new optimized DWC for Alcohol case study. The DWC configuration has only one column (S-101) which contains dividing wall in this column shell. The DWC has total 60 stages with 15 stages in top, 28 stages in middle and 17 stages in the bottom portion. The diameter of the DWC is 1.40 m.

For retrofitting purpose, the existing column S-100 from the conventional column system is used for DWC because diameter requirement of DWC is meet with first column (S-100) diameter. The column S-100 can be cut with upper section of 15 stages and lower section of 17 stages. A new dividing wall (middle) section with 28 trays will be prepared separately with diameter of 1.40 m and then installed with the remaining portions. In newly made

middle section, 28 trays in a semi-circle shape are installed on each sides of divided wall. The column which is not considered for retrofitting purposes, it can be further used for plant capacity increase purposes. Figure 6-1 represents the DWC and its technical data that is obtained by retrofitting the existing conventional two-column system. Analyze the heat duties of existing column heat exchangers with heat exchangers of new DWC for reuse purpose.

In this case study, existing reboiler and condenser can be reused for retrofitted DWC because the heat duties of these heat exchangers are near about the heat duty that is required for the new DWC. The economic evaluation results for retrofitting conventional column system to DWC for Alcohol application are presented in Table 6-1. These results are based on the simulation data that is obtained after retrofitting of conventional column to DWC. The piping system attached with the conventional column S-100 needs some modifications to change the piping route for DWC.

Table 6-2 shows the comparison of different distillation schemes for Alcohol application. In retrofitted DWC case, total cost represents the cost of new middle section and newly installed trays. From Table 6-2, it is noticeable that there is 36% savings in total utilities cost along with savings in capital cost by using DWC as opposed to conventional two-column system for same distillation process. DWC offers 27% savings in total annual cost (TAC) in comparison with conventional two-column system. These attractive results provides motivation to use DWC instead of conventional two-column system. For currently operational plants, retrofitting of existing conventional system to DWC could be carried out and results are also very promising. The results of retrofitting shows reduction in energy consumption as well as savings in the total operating cost and the total annual running cost

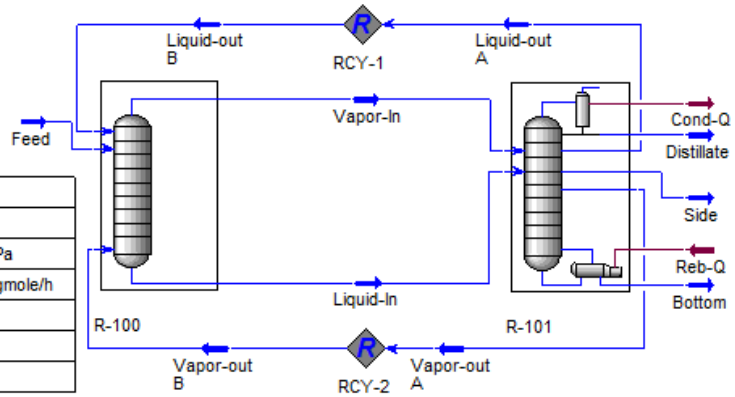
of the distillation column. Retrofitting of conventional two-column system to DWC offers more than 40% savings in total annual cost as opposed to conventional column system for this application.

Vapor-In		
Temperature	89.51	C
Molar Flow	104.0	kgmole/h
Master Comp Mole Frac (Ethanol)	0.2586	
Master Comp Mole Frac (1-Propanol)	0.7404	
Master Comp Mole Frac (1-Butanol)	0.0011	

Liquid-out B		
Temperature	89.88	C
Molar Flow	56.50	kgmole/h
Master Comp Mole Frac (Ethanol)	0.1220	
Master Comp Mole Frac (1-Propanol)	0.8774	
Master Comp Mole Frac (1-Butanol)	0.0006	

R-101		
Number of Trays	60.00	
Duties Summary (Condenser)	-1903	kW
Reflux Ratio	7.664	
Reboiler Duty	1921	kW

R-100		
Number of Trays	28.00	
Top Stage Press	87.54	kPa



Distillate		
Temperature	72.14	C
Molar Flow	20.22	kgmole/h
Master Comp Mole Frac (Ethanol)	0.9900	
Master Comp Mole Frac (1-Propanol)	0.0100	
Master Comp Mole Frac (1-Butanol)	0.0000	

Feed		
Temperature	93.95	C
Pressure	100.0	kPa
Molar Flow	100.0	kgmole/h
Master Comp Mole Frac (Ethanol)	0.2000	
Master Comp Mole Frac (1-Propanol)	0.6000	
Master Comp Mole Frac (1-Butanol)	0.2000	

Side		
Temperature	95.64	C
Molar Flow	60.54	kgmole/h
Master Comp Mole Frac (Ethanol)	0.0005	
Master Comp Mole Frac (1-Propanol)	0.9850	
Master Comp Mole Frac (1-Butanol)	0.0145	

Liquid-In		
Temperature	101.0	C
Molar Flow	156.0	kgmole/h
Master Comp Mole Frac (Ethanol)	0.0001	
Master Comp Mole Frac (1-Propanol)	0.8067	
Master Comp Mole Frac (1-Butanol)	0.1932	

Vapor-out B		
Temperature	101.0	C
Molar Flow	103.5	kgmole/h
Master Comp Mole Frac (Ethanol)	0.0001	
Master Comp Mole Frac (1-Propanol)	0.9011	
Master Comp Mole Frac (1-Butanol)	0.0988	

Bottom		
Temperature	121.2	C
Molar Flow	19.24	kgmole/h
Master Comp Mole Frac (Ethanol)	0.0000	
Master Comp Mole Frac (1-Propanol)	0.0100	
Master Comp Mole Frac (1-Butanol)	0.9900	

Figure 6-1: Results of Retrofitting Conventional Distillation System to DWC: Alcohol Application

Table 6-1: Economic Evaluation of Retrofit-DWC: Alcohol Application

Description	**Retrofitted Divided Wall Column**
Economics Detail	
Reboiler Duty (kW)	1921
Condenser Duty (kW)	1903
Total Stages	60
Column Diameter (m)	1.40
Column Height (m)	45
Area of Condenser (m^2)	101.24
Area of Reboiler (m^2)	55.06
Installed Cost	
Column Shell Cost (US$)	477429
Column Trays Cost (US$)	30245
Column Condenser Cost (US$)	0
Column Reboiler Cost (US$)	0
Total Installed Cost (US$)	507674
Utilities Cost	
Unit Cost of Cooling Water (US$/$m^3$)	0.073
Cooling Water Cost (US$/yr)	99031
Unit Cost of Steam (US$/Ton)	17.01
Steam Cost (US$/yr)	484774
Total Operating Cost (US$/yr)	583805
Total Annual Cost (US$/yr)	**753030**

Table 6-2: Economic Evaluation of Different Distillation Schemes: Alcohol Separation

Description	**Conventional Two-Column system**			**Divided Wall Column**	Savings (%)	**Retrofit-DWC**
Economic Details	S-100	S-101	Total	S-101		R-101
Reboiler Duty (kW)	1876	1144	3020	1927	36	1921
Condenser Duty (kW)	1873	1128		1909		1903
Total Stages	32	27		60		60
Column Diameter (m)	1.4	1.1		1.4		1.4
Column Height (m)	22.2	19.2		45		45
Column Volume (m^3)	39.9	20		79.4		79.4
Area of Condenser (m^2)	68.33	59.34		101.24		101.24
Area of Reboiler (m^2)	53.6	32.69		55.06		55.06
Installed Cost						
Column Shell Cost (US$)	522844	359879		922274		477429
Column Trays Cost (US$)	33911	20181		68739		30245
Column Condenser Cost (US$)	206948	188816		267204		0
Column Reboiler Cost (US$)	210816	152868		214531		0
Total Installed Cost (US$)	974519	721744		1472748		507674
Utilities Cost						
Unit Cost of Cooling Water (US$/$m^3$)	0.073	0.073		0.073		0.073
Cooling Water Cost (US$/yr)	97469	58700		99343		99031
Unit Cost of Steam (US$/Ton)	17.01	17.01		17.01		17.01
Steam Cost (US$/yr)	473418	288694		486288		484774
Total Operating Cost (US$/yr)	570887	347394	918281	585631	36	583805
Total Annual Cost (US$/yr)	895727	587975	**1483702**	**1076547**	**27**	**753030**

6.2 Results and Discussion

Results of retrofitting a conventional two column distillation system to DWC is presented in details in previous section. Alcohol mixture case study was selected from the literature and retrofitting procedure was successfully applied on the selected application. After applying retrofitting procedure, results shows that operating cost and capital investment can be lowered. These results also shows the importance and benefits of DWC for new plants. Table 6-3 presents the analysis summary including details of utilities cost, heat duties and capital cost for different column configurations of all case studies selected for this research.

The overall analysis shows attractive savings and less energy requirements in retrofitting procedure due to its operational advantages. For any application where retrofitting of operational column to DWC is not beneficial or there is less savings in the capital cost, then some alternative solution can be utilized to improve the savings in investment cost.

Table 6-3: Overall Performance Analysis of Different Distillation Schemes for all Case studies

Application	Distillation Column Scheme	Reboiler Duty (kW)	Installed Cost (US$/yr)	Utilities Cost (US$/yr)	Energy Savings (%)
Aromatics Separation	Conventional column system	2230	1313642	691907	
	DWC	1345	1115822	417687	39
Alcohols Separation	Conventional column system	3020	1696263	918281	
	DWC	1927	1472748	585631	36
	Retrofitted DWC	1921	507674	583805	
Alkanes Separation	Conventional column system	705	1016237	212985	
	DWC	472	782947	142634	33

6.3 Scope of Research in Kingdom of Saudi Arabia

Saudi Arabia is amongst the world's largest producer and exporter of petroleum products. After Russia, Saudi Arabia is leading crude oil producer country. Due to this massive production of petroleum products and export to other countries, economy of the Kingdom is directly dependent on oil sector including petroleum refineries and petrochemical industries. Saudi Arabia has 18% of world's proven petroleum reservoirs and about 92% of budget revenues are related to petroleum sector. The petroleum industry in Kingdom is growing very rapidly and this significant expansion of petroleum sector will contribute huge revenue to the economy of the Kingdom in future. Distillation is the main part of any process industry. Its high energy consumption directly affects the profit and business of any leading company. Implementation of DWC could reduce energy consumption (operating cost) and total annual cost significantly as opposed to the conventional multi-components distillation column arrangement.

The innovation in DWC technology will be very helpful and beneficial to all the industries in Saudi Arabia by implementing new DWC structure and also by retrofitting the conventional existing column to divided wall column.

All the process industries in the Kingdom need this new DWC technology to get maximum profit by minimizing energy and total annual cost. CO_2 emission is very hot issue in process industries now days and Environmental Protection Agencies (EPA) also working to keep the environment green and clean, so implementation of DWC in process industries will helpful in reducing the CO_2 level in atmosphere. Leading Companies in Kingdom like

Saudi Aramco, SABIC, Yanbu National Petrochemical Co., and Petro Rabigh etc can get direct advantages from new technology of divided wall distillation column.

6.4 Future Recommendations

In terms of technology innovation, it is necessary to continuously working to improve the DWC structure for energy saving. In this study, the optimal design aspect has been analyzed for the improved DWC structure to enhance performance. Future recommendations regarding this research are as follows.

- Setup of pilot scale plant of three products divided wall column in Chemical Engineering Department laboratory to validate the simulation results experimentally.
- Development of advanced control strategy Model Predictive control (MPC) for three products DWC and this could be based on extensive dynamic simulation study.
- Development of standard model of three product DWC in HYSYS simulator.

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2. **Bashir S.**, Al-Shammari A., Shamsuzzoha M., Design of Three Product Divided Wall Column, Poster presentation, 3rd Middle East Process Engineering Conference (MEPEC), Kingdom of Bahrain, September 2015
3. Shamsuzzoha M., **Bashir S.**, Al-Shammari A., Al-Mutairi E., Design and Control Strategy of the Divided Wall Column for Energy Saving, Poster presentation, The National

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